

**Part 1: Development of a Full-Congener Version of EPA Method
1668 and Application to Determination of 209 CB Congeners in
Aroclors**

and

Part 2: Development of EPA Method 1668A

by

Brian Fowler
Axys Analytical Services Ltd
Sidney, BC
Analytical@axys.com

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Summary

Part 1 of this report gives results of a study to expand EPA Method 1668 for determination of 209 chlorinated biphenyl (CB) congeners, and presents results of analyses of Aroclors using the expanded method. Part 2 of this report gives details supporting Revision A of EPA Method 1668 (Method 1668A). The work supporting Part 1 was conducted in early- to mid-1998; the work supporting Part 2 was conducted in 1999.

Part 1 of this report

The basic version of EPA Method 1668 (Reference 1) was developed by EPA and published in 1995 for determination of the 13 polychlorinated biphenyl (PCB) congeners established as toxic in 1994 by the World Health Organization (WHO; Reference 2). The identity and concentration of the "toxic" congeners is determined by high resolution gas chromatography combined with high resolution mass spectrometry (HRGC/HRMS).

The Part 1 study focused on HRGC separation and HRMS detection of the 209 congeners, consistent with a reasonable analysis time and a defined level of quality control (QC). The resulting expanded method used five solutions of congeners that, when analyzed individually, allowed separation and establishment of retention time and other data for all 209 CB congeners.

Details of the expanded method are given in Tables at the end of this Part 1. Data include compositions of stock and individual congener solutions, HRGC and HRMS operating conditions, HRMS targeting parameters and ion abundance ratios, GC retention times (RTs) and relative retention times (RRTs), and MS response factors (RFs). Using the analytical conditions developed in this study, approximately 135 of the 209 CBs are resolved with less than a 40% valley between the nearest-eluted congener on an SPB-Octyl column, and by using both SPB-Octyl and DB-1 columns, more than 165 individual congeners are resolved. Using ion source conditions that minimize fragmentation and mass resolution of 10,000, interference of co-eluting higher chlorinated homologues was found to be minor.

The 11 common Aroclors were analyzed for individual congener concentrations for resolved congeners and for homologue group totals. Concentrations found using the expanded method agree well with published values.

Part 2 of this report

Part 2 involved optimizing the operating conditions for determination of the 209 congeners as individual congeners and congener groups on the SPB-Octyl GC column. The objective was to focus Revision A of Method 1668 (Method 1668A) on analysis of environmental samples using a single HRGC/HRMS run, thereby maintaining a reasonable cost for the analysis.

The quantitation scheme was refined and standardized to focus all performance tests (multi-point calibration; calibration verification; initial precision and recovery; on-going precision and recovery; and labeled compound recovery from blanks and samples) on the 12 congeners presently designated as toxic by WHO (Reference 3) and the first- and last-eluted congener at each level of chlorination (LOC).

Performance testing at each LOC assures that reliable measurements can be demonstrated at each LOC.

Estimated method detection limits (EMDLs) and estimated minimum levels of quantitation (EMLs) were established for all congeners based as the mean plus two standard deviations of results of analyses of approximately 30 blanks (aqueous, soil, and tissue).

QC acceptance criteria were added and revised to cover the 12 WHO congeners, the LOC congeners, and the $^{13}\text{C}_{12}$ -labeled congeners in all performance tests.

Part 1: Development of a Full-Congener Version of EPA Method 1668 and Application to Determination of 209 CB Congeners in Aroclors

Introduction

The October 1995 version of EPA method 1668 is congener-specific for determination of a suite of 13 toxic PCB congeners by high resolution GC coupled with high resolution MS using $^{13}\text{C}_{12}$ -labeled PCBs as reference compounds for identification and quantitation. The targeted congeners included 3 non-ortho substituted co-planar PCBs, 8 mono-ortho substituted PCBs, and 2 di-ortho substituted PCBs. EPA Method 1668 is modeled closely after high resolution MS methods for polychlorinated dibenzo-*p*-dioxins and dibenzofurans such as EPA Method 1613 (Reference 4). These methods require the MS to be operated in mass locked, selected ion monitoring (SIM) mode with quantitation against a suite of $^{13}\text{C}_{12}$ -labeled compounds. The methods offer very high sensitivity and selectivity, and the extensive QC procedures lead to high quality data. Accordingly, EPA Method 1668 is both highly sensitive and selective, and produces reliable, high quality results when samples are analyzed for the targeted PCB congeners. Determination of the 13 toxic congeners is generally conducted on a single extract that invariably includes many other CB congeners. As human health risk assessment decisions call for determination of total CBs (Reference 5) or homologue totals, expansion of Method 1668 to allow determination of all 209 CB congeners is desirable. This report gives details of the tests performed and analytical conditions necessary to expand the Method to a full congener version and to apply the expanded version of the Method to determination of 209 congeners in a 11 Aroclors.

Analytical standards

Native and labeled congener standards

Two sets of standards containing 209 CB congeners were formulated and prepared by AccuStandard Inc., New Haven, CT. These native congener standards were used with a suite of $^{13}\text{C}_{12}$ -labeled compounds formulated and prepared by Cambridge Isotope Laboratories, Andover, MA (CIL). The $^{13}\text{C}_{12}$ -labeled compounds included the labeled analogues of the 13 target 1994 WHO toxic PCB congeners, nine labeled analogues of selected tetra- though hepta-CB congeners, four labeled injection internal standards (one for each chlorination level of the target congeners), two labeled clean-up standards, and labeled decachlorobiphenyl.

To cover the wider range of congeners in the expanded method, five additional $^{13}\text{C}_{12}$ -labeled congeners were added to the labeled spiking standard, one for each chlorination level not covered by the targeted congeners. The labeled congener standard was prepared from five individual $^{13}\text{C}_{12}$ -labeled congener stock solutions supplied by CIL. Labeled compounds employed in the full congener method and those used in the original Method are listed in Table 1.

Congeners are identified throughout this report using the IUPAC congener numbers as derived by Guitart, *et al.* (Reference 6). The IUPAC and Ballschmitter-Zell (BZ) numbering systems are similar but differ for six congeners: IUPAC congeners 107, 108, 109, 199, 200 and 201 correspond to BZ# 108, 109, 107, 201, 199 and 200, respectively.

A set of four mixtures of PCB congener standards (CLB-1 standards, from National Research Council of Canada (NRC), Marine Analytical Chemistry Standards Program, Halifax, Nova Scotia, Canada) containing 51 congeners were used for partial confirmation of peak assignments. Sources of the eleven Aroclor standards analyzed by extended Method 1668 are indicated in Table 2.

Formulation of full congener standards

Standards containing all 209 congeners were formulated to allow establishment of GC retention times. The goal was a set of standards that would allow each CB to be fully resolved from all others on an SPB-Octyl column. The formulation was based on the relative retention time (RRT) database published by George Frame (Reference 7), who generously provided an electronic copy of the database as an Excel spreadsheet file. To predict retention times for data to be acquired for this project, the RRT database for a 30-m SPB-Octyl column coupled to an MS detector (database system 7, contributed by N. Erwin of Supelco) was used. Congeners listed in the database and sorted by IUPAC congener number were resorted first by chlorination level then by RRT on the SPB-Octyl column, then allocated to five standard mixtures, designated A through E.

The initial set of five standards was formulated with 41 to 42 congeners in each solution. Subsequently, five custom standard mixtures were prepared from individual high-purity (typically >99.5%) congener standards by AccuStandard (Reference 8), and provided at a concentration of 500 ng/mL in iso-octane. An aliquot of each stock was spiked with the $^{13}\text{C}_{12}$ -labeled compounds and extended internal standards (Table 1) to produce solutions with the native congeners and labeled compounds at concentrations of 50 and 100 ng/mL, respectively. Each of these solutions was analyzed by HRGC/HRMS using procedures described below.

Congener assignments were checked by analysis of other individual congener standards including the NRC CLB-1 series, by comparison to available labeled congeners, and to congeners present in the regular Method 1668 standards. Unambiguous retention time assignments were possible for 208 individual congeners under extended Method 1668 conditions. The 2,2',3,4,4'-pentachloro congener (IUPAC #85) was absent from the initial set. The omission was subsequently confirmed by AccuStandard.

For the 208 congeners, the observed retention times agreed well with the predicted values. The mean difference of determined retention time from expected retention time was 6.0 s (relative standard deviation of 0.32%). Formulation errors resulted in co-elution or incomplete separation of four pairs of isomeric congeners. Subsequently, a second set of standards (Series 2 standards, A2 to E2) were formulated to be fully resolved on the SPB-Octyl column under extended Method 1668 conditions using a criterion of the valley between resolved congeners to be less than 2%. This conservative separation criterion was adopted to allow for inter-column variability such that these standards would be expected to be well resolved on a range of 30-m SPB-Octyl columns. Runs of these standards also allowed calculation of relative responses for isotope dilution quantitation and of response factors for internal standard quantitation.

The "Series 2" standards were formulated using retention times determined using the initial set of assignment standards run on the SPB-Octyl column. A calculated retention time was used for CB 85, the penta congener omitted from the initial standards. The five "Series 2" custom standards contained from between 15 to 82 congeners and were supplied at concentrations of 250 $\mu\text{g}/\text{mL}$ for the mono- to tri-CBs; 500 $\mu\text{g}/\text{mL}$ for the tetra- to hepta-CBs; and 750 $\mu\text{g}/\text{mL}$ for the octa- to deca-CBs. The concentrations increase with chlorination level in three steps to give similar instrument responses for all congeners. Standard A2 contains 83 components, the maximum number of non-window-defining congeners that are "fully" resolved on the SPB-Octyl column. Standards B2, C2, and D2 included congeners incompletely resolved from congeners in the A2 standard, and the E2 standard contained primarily the window-defining congeners.

Window-defining congeners, defined as the first and last eluters of each homologue group, are characteristic of the stationary phase in a given GC column. For the two columns used in Method 1668 and this study, the same congeners form the window-definers. It should be noted that the window defining mix for a DB-5 column that is supplied by CIL (PCB Window Standard for DB-5, Cat # EC-

1430) is formulated with three components different than components formulated for the SPB-Octyl and DB-1 columns. The difference in retention times for these alternate components is generally minor except for the first eluting trichloro isomer (congener 19) that elutes almost 2 minutes earlier than the first trichloro isomer (#30) in the CIL window-defining standard for the DB-5 column. Using the CIL EC-1430 standard, congener 19 could easily be missed as the first-eluting trichloro isomer on the SPB-Octyl and DB-1 columns.

The composition of the Series 1 and Series 2 standards is given in Tables 3a and 3b, respectively. The window-defining congener RRTs and typical retention times for the SPB-Octyl and DB-1 columns are given in Table 4.

Working standards were prepared from the high concentration Series 2 stocks diluted by a factor of 5000 to 50 ng/mL (mono-CB to tri-CB), 100 ng/mL (tetra-CB to hepta-CB) and 150 ng/mL (octa-CB to deca-CB). These levels correspond broadly to the calibration verification (CS-3) standard in Draft Method 1668. Five individual retention time calibration standards, each fully resolvable on the SPB-Octyl column, were prepared using an aliquot of the each of the Series 2 stock solutions, and a full-congener standard was prepared by combining an aliquot all five of the Series 2 standards. The set of calibration standards included the full suite of $^{13}\text{C}_{12}$ -labeled congeners for expanded Method 1668, (Table 1).

Instrumental analyses

Analytical instruments

Analyses were conducted on two Micromass high resolution mass spectrometer systems: a VG 70 VSE with DEC VAX 3100 workstation and an Autospec Ultima Series V with DEC VAX 4000/60 workstation. Each MS was coupled to a Hewlett Packard 5890 Series II gas chromatograph with CTC A200S autosampler and the GCs were equipped with a split/splitless injector, silanized double gooseneck injector liner and 5-m deactivated silica guard column with Restek Press-fit connector.

GC columns and conditions

The GC injector was run at 280 °C. The column was operated in constant pressure mode at a head pressure of 100 to 120 kPa with ultra-high-purity (UHP) helium as carrier gas. Injections of 1.0 μL were made in splitless mode with inlet purge resumed after 2 minutes. The primary columns were SPB-Octyl (50% octyl-50% polydimethylsiloxane, Supelco) and DB-1 (100% polydimethylsiloxane, J&W Scientific), each 30 m x 0.25 mm ID, 0.25 μm film, fused-silica, bonded-phase capillary column, coupled directly to the MS ion source. GC conditions were modified from those in Method 1668 to programs similar to those used in the retention database. Compared to the recommended Method 1668 conditions, the GC programs used provided improved separation of lower chlorinated congeners and simplified mass scan descriptor setup with a minor increase in GC run time. Under typical conditions the measured peak widths at half height for congeners 52 and 180 were 3.5 to 4.5 seconds, respectively. GC temperature programs used and other operating conditions are given in Tables 5a and 5b for the SPB-Octyl and DB-1 columns, respectively.

HRMS conditions

Mass spectrometer conditions were modified from the Method 1668 conditions to include the exact m/z's of three most abundant m/z's from the parent ion clusters of mono- to deca-CB and two exact m/z's for the $^{13}\text{C}_{12}$ -labeled analogs. The HRMS instruments were operated in the selected ion V-SIR mode, in which each exact m/z is monitored by simultaneously stepping the acceleration and deflection voltages at constant magnetic field. In this mode, the range of m/z's scanned at any time is limited to less than a

factor of two. Beyond this range, ion transmission and mass resolution degrade. To minimize the range scanned at any given time, limited mass ranges were scanned in six groups (functions), each function at constant magnetic field. These conditions reduce the maximum to minimum mass range scanned to less than a factor of 1.4.

All analyses were conducted at starting acceleration voltage of 8 kV. For approximately 2 seconds at the start of each function in the V-SIR mode, no useful data are collected. Therefore, the function switch points were carefully positioned at times during which it was known that no congener would elute. Consequently, different scan functions and switch points were used for the SPB-Octyl and DB-1 columns. The scan descriptors and function boundary switch points were established as to acquire the native and $^{13}\text{C}_{12}$ -labeled CB congeners for each level of chlorination. These descriptors are given in Tables 6a and 6b for the SPB-Octyl and DB-1 columns, respectively and the distribution of homologue groups monitors in each function for these scan descriptors is summarized in Table 6c.

The MS instruments were tuned daily for maximum response at mass resolution of 10,000 and mass calibrated against perfluorokerosene (Fluka Chemicals). As part of the daily mass calibration procedure prior to sample analysis, mass resolution and peak shape were recorded for a set of significant PFK fragment ions covering the mass range of the scan function. During mass calibration, mass peak width was recorded to verify 10,000 mass resolution over the mass range scanned.

The HRMS instruments were operated at an ion source temperature of 200 °C and electron energy of 40 eV. The relatively low ion source temperature and low energy ionization reduce fragmentation and promote parent ion formation. These conditions minimize interference from fragments of higher homologues.

Mass chromatograms were printed using automated methods (OPUS command files) and quantitated using OpusQUAN database quantitation software (Version 2.0, MicroMass, UK) run on the VAX data systems and a DEC Alpha 433 workstation. OpusQUAN analyte tables summarizing key targeting parameters (target compounds, retention times, calibration and quantitation references, location windows, isotope ratios, etc.) for the SPB-Octyl and DB-1 columns are given in Tables 7a and 7b, respectively. The OpusQUAN analyte tables for each column type are presented in four parts. This simplification was required to facilitate execution of full congener quantitation methods on less powerful VAX systems. The OpusQUAN form limits were expanded to allow quantitation of up to 250 target analytes.

Quantitation and identification procedures

The isotope dilution method was used for quantitation of each native CB for which a $^{13}\text{C}_{12}$ -labeled analog is added prior to sample preparation. All other CBs were quantified by the internal standard technique using the closest-eluted $^{13}\text{C}_{12}$ -labeled compound added prior to extraction as reference. This approach provides recovery-corrected data for all CB congeners.

The $^{13}\text{C}_{12}$ -labeled compounds, including the cleanup standards, were quantified by the internal standard technique using the closest-eluted injection internal standard as reference.

Individual CB congeners were located using retention time relative to the nearest-eluted $^{13}\text{C}_{12}$ -labeled compound within a 6 to 10 second (± 3 to ± 5 sec) retention time window. The OpusQuan targeting method calculated the ion abundance ratio for each targeted congener and flagged those meeting the $\pm 15\%$ tolerance criterion. A sample-specific detection limit was calculated based on 4 x total mass channel noise, the channel noise being measured at the start of each function unless specified otherwise. Theoretical ion abundance ratios and QC limits are given in Table 8.

Results and Discussion

Analysis of the custom Series 2 congener standards

Retention time data on the SPB-Octyl column and separation between congeners for each of the five Series 2 standards are presented in Table 9a, sorted by retention time for each level of chlorination. Retention time data for all 209 congeners sorted by level of chlorination then retention time are given in Table 9b. Although absolute retention times are presented in these tables, they are simply typical observed values and should not be expected to be reproduced exactly. The congener elution order, peak separations, and relative retention times are more important. The closest separations observed for the Series 2 standards are 14 seconds between penta-CBs 87 and 119 in standard A2 and tetra-CBs 65 and 59 in standard C2. Table 3b summarizes the composition of the Series 2 standards. Separation of all 209 congeners is possible in three or four mixtures, but with fewer mixes, some components are only partially separated with a 50% valley. Critical regions on the SPB-Octyl column occur around 37 minutes for the penta-CBs, where six congeners (108, 119, 86, 97, 125 and 87) elute in a 14-second window and at 44 minutes where four hexa-CBs (163, 138, 129 and 160) elute in a 9-second window.

Under the conditions described above, the SPB-Octyl column separates the 209 congener standard into 165 peaks (domains), and resolves 135 congeners as individual peaks separated by a valley of 40% or less. Analysis of the full congener calibration standard 209 on both the SPB-Octyl and DB-1 columns resolves 166 individual congeners.

Although the SPB-Octyl column shows excellent specificity and efficiency for this analysis, this column type is not without problems. The recommended maximum isothermal temperature is 280 °C but in order to elute all PCB congeners in a practical time, the column is programmed to 290 °C which leads to progressive loss of stationary phase. This phase loss in turn causes progressive shifts in retention time shifts which are compensated by daily head pressure adjustment. Bleed pulses from a new SPB-Octyl column can result in erratic lock-mass response and poor source performance and can be reduced by conditioning the column for several hours before use. The SPB-Octyl stationary phase appears to be very sensitive to oxygen and when oxidized, bleed levels increase and changes in congener elution order are evident. Resolution of Cl-3 congeners 34 and 23 is used as a measure of column performance. These congeners are separated by 9 or 10 seconds on a column in good condition. Separation of congeners 156 and 157 is another indication of column condition as these congeners co-elute on an SPB-Octyl column in good condition, and become resolved with phase loss or oxidation.

Based on the first two Octyl columns used for this work the following preliminary GC performance specifications were adopted:

1. The column must resolve Cl-3 congeners 34 and 23 (Figure 1) and Cl-8 congeners 187 and 182 (Figure 2) with a maximum valley 40%
2. Cl-6 congeners 156 and 157 should not be resolved and co-elute or elute within 2 seconds at peak maximum
3. Retention time of PCB 209 should exceed 55 minutes.

Supelco has subsequently supplied SPB-Octyl columns pre-selected to meet this performance specification.

Retention time data and separations on the DB-1 column for the Series 2 standards are presented in Table 10a. Eight congeners in the Series 2 standards co-elute on DB-1. Retention times for all 209 sorted by level of chlorination then retention time on DB-1 are given in Table 10b.

Response factors (RFs) relative to the closest eluting $^{13}\text{C}_{12}$ -labeled congener for all congeners were determined using the Series 2 standards on the SPB-Octyl column. RFs for all congeners are listed in Table 11a and summarised in Table 11b. RFs range from 0.44 to 1.35 but are typically in the range 0.8 to 1.2.

Aroclor analysis

The quantity of each Aroclor taken for full congener analysis was determined such that concentration of the most abundant congener was at 2000 ng/mL, this being the calibration upper concentration limit, equal to the concentration of the CS-5 standard in the set of calibration standards in original Method 1668. Levels of the most abundant congener (MAC) in each Aroclor were taken from George Frame's paper (Reference 9) on semi-quantitative Aroclor congener distributions. The MACs, the MAC levels, and quantities of Aroclor taken are given in Table 12. The small Aroclor sample size ensures the MACs are within linear range but also raises the detection limit for the trace components. It should be noted here that the upper concentration limit of calibrated range in the Draft Method is substantially lower than the actual working upper limit of the HRMS instrument. The instrument upper working concentration allows higher level linearity standards by up to an order of magnitude higher than older instruments (e.g. a Micromass 70-VSE). This greater range, combined with the higher sensitivity of newer instrumentation (e.g. a Micromass AutoSpec Ultima) provide a working calibration range up to two orders of magnitude greater than in the original Method.

Aroclor samples were quantitated for the set of resolved GC peaks (domains) for each column using RF's and retention times derived from a the combined standard containing all 209 congeners. Calibration of the 209 congener standard used a single point calibration.

Eleven Aroclors were analyzed by the expanded method, but only detailed results for Aroclor 1254 and summary data for other selected Aroclors are presented in the body of this report to conserve space. The composition of Aroclor 1254 as weight percent is tabulated in Tables 13 and 14 for the SPB-Octyl and DB-1 columns, respectively. The Tables include retention times (RTs) and ion abundance ratios (RAs) for the GC domains defined by the full congener calibration standard and a detection limit based on ion channel noise. Components detected within the 15% tolerance RA limit are qualified with a "y," otherwise marked "n." The retention time of detected peaks is listed in minutes and seconds except where no peak is detected in one or both of the targeting ion channels, when the "Not Fnd" (i.e. not found) comment is entered.

By combining data from both columns, concentration in weight percent of congener resolved on either column can be determined and this is listed by congener in Table 15. Using a 50% valley separation criterion (after one smoothing pass), it was found that 166 congeners are resolved on at least one column. The data from the two columns are combined in a MicroSoft Excel spreadsheet to automate selection of the appropriate column, avoid duplicate reporting of unresolved components and carry out some de-convolution of unresolved compounds. Reporting off the two columns increases the specificity of the method but also adds complexity to data reduction. Several congeners are unresolved on both columns although in some cases contributions from other components may be subtracted. For instance CB 160 co-elutes with 138, 163, and 129 on SPB-Octyl and with 158 on DB-1 but, as 158 is resolved on Octyl, the difference between the DB-1 158+160 and Octyl 158 provides the 160 concentration.

In those cases where a congener is resolved on both columns, the concentration from the SPB-Octyl column is reported, although a mean or even minimum value could also be calculated. Co-eluting congeners listed more than once would result in over-estimation of CB totals and summing errors in homologue totals. Where co-elutions of a specific congener occur on both columns, a total concentration of co-eluting congeners is listed only for the most abundant congener. Abundance data for the co-eluting congener group is based on data from references 9 and 10. The congener used to report summed components is indicated on the lines for the other components. For instance, the dichloro congeners 12 and 13 co-elute on both SPB-Octyl and DB-1, and the detected total 12+13 is reported on the CB 13 line and a reference is made for CB 12 to "see 13." Although attention was paid to avoid duplicate congener

contribution, at this time there remain some cases that may lead to a some over-reporting in homologue totals.

Data for the resolved congeners found in Aroclor 1254 are compared to published data in Table 15 and indicate reasonable agreement to the Schultz *et.al.* data (Reference 10), with some significant differences from the data from Frame's laboratory (Reference 9). These data suggest that the Aroclor 1254 used to test expanded Method 1668 may differ in composition from that used by Frame and is likely closer to the Aroclor tested by Schulz *et.al.* The differences are most pronounced for congeners 52, 66, 49, 118 and 151. Compositional differences between batches for 1254 have been noted previously by Frame.

Results for Aroclor 1221, 1016, 1232, and 1248 are presented in Appendix A in the same format as Table 15. Congener concentrations are reported in wt % (i.e. ng/100 ng of Aroclor) and each are compared to data reported by Schulz *et.al.* (Reference 10) and Frame (Reference 9). These results should be considered preliminary and were produced without detailed review or manual intervention and used the nominal design concentrations of standards. They are presented here to demonstrate the utility and power of the method. It is expected that accuracy will improve by the normal iterative QC process is applied. The refinements described in the following section should also lead to improved method performance.

Conclusions

The expanded method allows reporting of results for 166 individual congeners when both the SPB-Octyl and DB-1 columns are used; the remaining 43 congeners are included as components of unresolved peak domains. Using only the SPB-Octyl column, the 209 congeners are resolved into 165 peaks with resolution of 135 individual congeners.

Part 2: Development of EPA Method 1668A

Introduction

Development of the expanded version of EPA Method 1668 in Phase 1 of the study focused on establishment of analytical conditions necessary for HRGC separation and HRMS detection of the 209 congeners, consistent with a reasonable analysis time and a defined level of quality control (QC). Based on Phase I study data, EPA produced a draft version of EPA Method 1668, Revision A (Method 1668A). Draft Method 1668A contained fixed estimates for QC acceptance criteria for the QC performance tests. These estimates were based on preliminary data. In addition, draft Method 1668A lacked estimated method detection limits (EMDLs) and estimated minimum levels of quantitation (EMLs) for all congeners except the 13 congeners originally designated as toxic by WHO (Reference 2). EPA evaluated results of the Phase 1 work and, in the fall of 1999, conducted a peer review of draft Method 1668A. Based on the evaluation and peer review, EPA determined that missing details needed to be filled in to support widespread application of Method 1668A. This Part 2 of this report describes development of those details.

Addition and re-arrangement of labeled compounds

Part 1 of this report described the addition of at least one $^{13}\text{C}_{12}$ -labeled compound at each level of chlorination (LOC) for identification and quantitation of the 209 CBs. The expanded list of labeled compounds was incomplete, in that the first- and last-eluted $^{13}\text{C}_{12}$ -labeled compound at each LOC was not included, and labeled compounds were included that were neither the first- nor last-eluted compound. In discussions with Cambridge Isotope Laboratories (CIL), CIL agreed to synthesize the missing labeled compounds. Also, $^{13}\text{C}_{12}$ -labeled analogues of toxic congeners 123 and 114 have become available since the draft method was released. The new standards allowed re-arrangement of the available labeled compounds for use as additional cleanup standards and injection internal standards.

Addition of $^{13}\text{C}_{12}$ -labeled window-defining congeners

Data on method performance for a wide range of congeners is provided by the addition of the $^{13}\text{C}_{12}$ -labeled LOC/window defining congeners. These congeners also define the retention time window at each LOC for every instrument run. So that all congeners at a given LOC can be monitored in each HRGC/HRMS run, the list of $^{13}\text{C}_{12}$ -labeled compounds was expanded to include the first- and last-eluted congener at each LOC. The complete list of $^{13}\text{C}_{12}$ -labeled congeners that define the window at each LOC is given in Table 16.

Addition of $^{13}\text{C}_{12}$ -labeled cleanup standards

The expanded version of Method 1668 used $^{13}\text{C}_{12}$ -labeled CB 111L as a cleanup standard. Adding the window-defining congeners allowed $^{13}\text{C}_{12}$ -labeled CBs 28L and 178L to be used as additional cleanup standards. The list of cleanup standards is shown in Table 16.

Addition of $^{13}\text{C}_{12}$ -labeled injection internal standards

The $^{13}\text{C}_{12}$ -labeled LOC/window-defining congeners and $^{13}\text{C}_{12}$ -labeled cleanup standards are located in each HRGC/HRMS run by reference to $^{13}\text{C}_{12}$ -labeled injection internal standards. However, the GC run covers a broad retention time (RT) range of approximately 10 to 55 minutes. Colby *et.al.* (Reference 11) have shown that a target compound is most accurately identified if its retention time relative to its reference compound is in the range of 0.8 to 1.2. To attempt to limit the RRTs for the $^{13}\text{C}_{12}$ -labeled LOC/window-defining compounds to this range, the list of $^{13}\text{C}_{12}$ -labeled injection internal standards was

expanded to five congeners with IUPAC numbers 9L, 52L, 101L, 138L, and 194L. The list is shown in Table 16.

Expansion of calibration

In the October 1995 version of Method 1668, a 5-point calibration was employed for the 1994 list of WHO toxic congeners. For Method 1668A, the addition of $^{13}\text{C}_{12}$ -labeled LOC/window-defining congeners allowed establishment of 5-point calibration for the native analogs of these compounds.

To take advantage of the added sensitivity of high-sensitivity HRMS instruments a 6th calibration point was added at 1/5 the concentration of the lowest calibration level in the 5-point calibration. All native congeners are now at equal concentration at each calibration level, in contrast to the concentration steps within a level for the more abundant congeners stipulated for the original version of EPA Method 1668.

The compounds and concentrations required for multi-point calibration are listed in Table 17. Table 17 forms Table 5 of EPA Method 1668A.

Refinement of relative retention time links

Expansion of the list of $^{13}\text{C}_{12}$ -labeled LOC/window-defining compounds allowed refinement of the means of CB identification through RRTs. The final scheme arrived at was use of the nearest-eluted $^{13}\text{C}_{12}$ -labeled LOC/window-defining congener or $^{13}\text{C}_{12}$ -labeled WHO toxic congener as RRT reference for each CB; and nearest-eluted injection internal standard as reference for the $^{13}\text{C}_{12}$ -labeled LOC/window-defining congeners, the $^{13}\text{C}_{12}$ -labeled WHO toxic congeners, and the $^{13}\text{C}_{12}$ -labeled cleanup standards. Finally, the $^{13}\text{C}_{12}$ -labeled injection internal standards were referenced to 178L, and 178L was referenced to itself.

Using this scheme, the following hierarchy is used for analyte location in an HRGC/HRMS run:

1. 178L is located first.
2. The other four $^{13}\text{C}_{12}$ -labeled injection internal standards are located relative to 178L
3. The $^{13}\text{C}_{12}$ -labeled LOC/window-defining congeners, the $^{13}\text{C}_{12}$ -labeled WHO toxic congeners, and the $^{13}\text{C}_{12}$ -labeled cleanup standards are located relative to the nearest eluted $^{13}\text{C}_{12}$ -labeled injection internal standard.
4. Each CB is located relative to the nearest-eluted $^{13}\text{C}_{12}$ -labeled LOC/window-defining congener or $^{13}\text{C}_{12}$ -labeled WHO toxic congener.

The link for each CB and $^{13}\text{C}_{12}$ -labeled compound is shown in Tables 9a and 9b. These relationships are also shown in Table 18 which forms Table 2 of Method 1668A.

Quantitation references

In the same way that a scheme for location of each CB needed to be refined, the scheme for quantitation of each CB needed refinement. For each CB with a $^{13}\text{C}_{12}$ -labeled LOC/window-defining analog or WHO toxic analog, the $^{13}\text{C}_{12}$ -labeled analog is used as the quantitation reference. For each CB without a $^{13}\text{C}_{12}$ -labeled LOC/window-defining analog or WHO toxic analog, the mean (average) response at both exact m/z's for all $^{13}\text{C}_{12}$ -labeled LOC CBs and WHO toxic CBs at a given LOC is used as the quantitation reference. These links are shown in Table 18. Use of the mean response has two significant effects: (1) an interference at a given exact m/z will have a minor effect on the mean response because the response is averaged over all m/z's at each LOC, and (2) because the LOC CBs and WHO toxic CBs are spiked into each sample, the result for every CB is recovery corrected. This eliminates the disparity that can exist between the isotope dilution recovery correction and normal internal standard quantitation techniques in which recovery correction for sample preparation and cleanup processes is not performed.

Estimated method detection limits and estimated minimum levels of quantitation

EPA normally establishes method detection limits (MDLs) and minimum levels of quantitation (MLs) by performing an MDL study using the MDL procedure at 40 CFR 136, appendix B. Two complications mitigate against this approach when MDLs and MLs are to be developed for the CBs: (1) The large number of congeners would require a large number of sample preparations and injections. This large number is prohibitively expensive; (2) the ubiquitous nature of certain of the CBs causes elevation of detection and quantitation levels. The approach suggested by Ferrario *et.al.* (Reference 12) addresses these complications. This approach uses the mean level of a large number of blank measurements plus two standard deviations of these blank measurements to establish a detection level. For this study, and for the data in Table 18, 30 blanks measured over the course of several months were used. These blanks encompassed aqueous, solid and tissue samples. The means plus two standard deviations were used to construct estimated method detection limits (EMDLs).

The EMDLs were multiplied by three and then rounded to the number nearest to (1, 2, or 5) $\times 10^n$, where n is an integer, to form estimated minimum levels of quantitation (EMLs).

The EMDLs and EMLs are shown in Table 18 for aqueous samples, for solid and semi-solid samples, and for final extracts.

Quality control acceptance criteria

The October 1995 version of EPA Method 1668 contained QC acceptance criteria for the $^{13}\text{C}_{12}$ -labeled analogs of the 1994 list of WHO toxic congeners and a single cleanup congener only. Expansion of Method 1668 to Method 1668A necessitated development of QC acceptance criteria for the revised list of WHO toxic congeners and their $^{13}\text{C}_{12}$ -labeled analogs, for the native and $^{13}\text{C}_{12}$ -labeled LOC/window-defining congeners, and for the $^{13}\text{C}_{12}$ -labeled cleanup congeners. An initial estimate of these limits was made by first determining the standard deviation of recovery from 30 recovery measurements from reference matrices for aqueous, soil, and tissue samples (e.g., reagent water for the aqueous reference matrix). The standard deviation was multiplied by two to create an initial estimate of the standard deviation QC acceptance criteria for the initial precision and recovery (IPR) test. An initial estimate of the recovery QC acceptance criteria for the IPR test was constructed as ± 2 standard deviations above and below the mean recovery. The initial estimate of the ongoing precision and recovery (OPR) QC acceptance criteria was constructed by widening the IPR recovery QC acceptance criteria by 10 percent.

An initial estimate of the labeled compound recovery from samples was constructed as ± 2 standard deviations above and below the mean recovery from results of analyses of 10 samples each of water, soil, and tissue.

The initial estimates of the QC acceptance criteria were highly variable and were not consistent with each other. For example, the IPR and OPR recovery limits for the $^{13}\text{C}_{12}$ -labeled compounds from reference matrices were wider than the recovery limits from samples. As a result, fixed limits were established for QC acceptance criteria of a given type, and were adjusted to make all recoveries self consistent. The QC acceptance criteria given in Method 1668A are given in Table 19. Table 19 forms Table 6 of Method 1668A.

Conclusion

Addition of $^{13}\text{C}_{12}$ -labeled compounds at each level of chlorination and rearrangement of labeled compounds as cleanup standards and injection internal standards allow improved identification and quantitation of the CB congeners. These refinements were used to produce Revision A of Method 1668

(Method 1668A).

Method 1668A was proposed for use in "Standards for the Use and Disposal of Sewage Sludge" on December 23, 1999 (64 FR 72045).

References

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Table 1. Labeled PCBs Surrogates in Draft and full congener version Method 1668

Draft 1668		Full Congener 1668	
Labeled PCB Congener	IUPAC	Labeled PCB Congener	IUPAC
Surrogates			
$^{13}\text{C}_{12}\text{-3,3',4,4'\text{-TeCB}}$	77	$^{13}\text{C}_{12}\text{-4-CB}$	3
$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-PeCB}}$	105	$^{13}\text{C}_{12}\text{-4,4'\text{-DiCB}}$	15
$^{13}\text{C}_{12}\text{-2,3',4,4',5\text{-PeCB}}$	118	$^{13}\text{C}_{12}\text{-2,4,4'\text{-TrCB}}$	28
$^{13}\text{C}_{12}\text{-3,3',4,4',5\text{-PeCB}}$	126	$^{13}\text{C}_{12}\text{-3,3',4,4'\text{-TeCB}}$	77
$^{13}\text{C}_{12}\text{-2,3,3',4,4',5\text{-HxCB}}$	156	$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-PeCB}}$	105
$^{13}\text{C}_{12}\text{-2,3,3',4,4',5\text{-HxCB}}$	157	$^{13}\text{C}_{12}\text{-2,3',4,4',5\text{-PeCB}}$	118
$^{13}\text{C}_{12}\text{-3,3',4,4',5,5'\text{-HxCB}}$	169	$^{13}\text{C}_{12}\text{-3,3',4,4',5\text{-PeCB}}$	126
$^{13}\text{C}_{12}\text{-2,2',3,4,4',5,5'\text{-HpCB}}$	180	$^{13}\text{C}_{12}\text{-2,3,3',4,4',5\text{-HxCB}}$	156
$^{13}\text{C}_{12}\text{-2,3,3',4,4',5,5'\text{-HpCB}}$	189	$^{13}\text{C}_{12}\text{-2,3,3',4,4',5\text{-HxCB}}$	157
$^{13}\text{C}_{12}\text{-Deca-CB}$	209	$^{13}\text{C}_{12}\text{-3,3',4,4',5,5'\text{-HxCB}}$	169
		$^{13}\text{C}_{12}\text{-2,2',3,4,4',5,5'\text{-HpCB}}$	180
		$^{13}\text{C}_{12}\text{-2,3,3',4,4',5,5'\text{-HpCB}}$	189
		$^{13}\text{C}_{12}\text{-2,2',3,3',4,4',5,5'\text{-OcCB}}$	194
		$^{13}\text{C}_{12}\text{-2,2',3,3',4,5,5,6,6'\text{-NCB}}$	208
		$^{13}\text{C}_{12}\text{-Deca-CB}$	209
Clean-up Standards			
$^{13}\text{C}_{12}\text{-3,4,4',5\text{-TCB}}$	81	$^{13}\text{C}_{12}\text{-3,4,4',5\text{-TCB}}$	81
$^{13}\text{C}_{12}\text{-2,3,3',5,5'\text{-PeCB}}$	111	$^{13}\text{C}_{12}\text{-2,3,3',5,5'\text{-PeCB}}$	111
Internal Standards			
$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	52	$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	52
$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	101	$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	101
$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	138	$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	138
$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	178	$^{13}\text{C}_{12}\text{-2,3,3',4,4'\text{-TCB}}$	178

Table 2. Sources and lot numbers of Aroclor Standards taken for full congener PCB analysis

Aroclor	Supplier	Supplier Lot #	SC# (Lab stock #)
1221	Ultra Scientific	AM-2T	1068
1232	Cambridge Isotope Laboratories	9AT-107-1004	0085
1016	Ultra Scientific	A-0165	1067
1242	Ultra Scientific	G-0076	0721
1248	Ultra Scientific	I-85	1070
5442	Chem Service Inc.-Caledon	205-125A	2442
1254	Ultra Scientific	G-0041	1071
5460	Chem Service Inc.-Caledon	199-53A	2441
1260	Ultra Scientific	G-0478	0723
1262	Cambridge Isotope Laboratories	BE-1135	0031
1268	Cambridge Isotope Laboratories	BE-1136	0032

Table 3a. Composition of initial set (Series 1) of full congener standards

Standard ID AccuStandard ID	A S-4494-A	B S-4494-B	C S-4494-C	D S-4494-D	E S-4494-E
Congener	1	2	3	4	10
	9	7	6	5	8
	14	18	11	13	30
	19	17	12	15	27
	24	16	25	32	34
	23	29	36	31	20
	26	33	54	28	22
	21	53	50	37	45
	39	46	52	43	69
	38	73	49	44	47
	35	48	65	62	42
	51	59	40	63	64
	75	41	71	60	61
	57	72	68	104	66
	74	58	67	94	78
	55	70	76	95	77
	80	56	81	88	96
	79	98	103	84	100
	93	89	121	101	102
	91	90	113	86	92
	119	99	112	97	83
	117	125	108	110	87
	107	85 ¹	116	82	115
	124	111	123	120	152
	118	109	114	106	145
	136	127	126	122	144
	148	154	155	105	134
	151	143	135	150	142
	140	139	149	147	133
	165	132	131	141	168
	130	161	146	164	138
	129	160	153	169	163
	158	166	137	188	128
	184	159	162	176	156
	178	167	187	175	157
	185	181	173	182	179
	174	172	192	177	186
	202	180	170	171	183
	204	201	189	193	191
	197	199	200	190	198
	196	195	194	207	206
	203	208	205	209	
# congeners	42	42	42	42	41

1. Penta-CB 85 not found; omitted from stock
2. Congeners identified by IUPAC numbers.

Table 3b. Composition of Series 2 full congener standards for Method 1668

Standard ID AccuStandard ID	A2 S-4687-A	B2 S-4687-B	C2 S-4687-C	D2 S-4687-D	E2 S-4687-E
Congener	2	7	13	25	1
	10	5	17	21	3
	9	12	29	69	4
	6	18	20	47	15
	8	24	46	42	19
	14	23	65	64	16
	11	28	59	70	37
	30	22	40	102	54
	27	39	67	97	43
	32	53	76	115	44
	34	51	80	123	74
	26	73	93	134	56
	31	48	84	131	77
	33	62	101	163	104
	36	71	112	180	98
	38	68	86		125
	35	58	116		110
	50	61	109/107		126
	45	55	154		155
	52	60	147		138
	49	94	140		169
	75	100	146		188
	41	91	141		189
	72	121	164		202
	57	90	158		205
	63	99	182		208
	66	108/109	174		206
	79	117	173		209
	78	111	193		
	81	107/108			
	96	118			
	103	114			
	95	150			
	88	145			
	89	135			
	92	149			
	113	139			
	83	132			
	119	165			
	87	168			
	85	137			
	82	160			
	120	128			
	124	162			
	106	157			
	122	184			
	105	186			
	127	187			
	152	185			

Table 3b. (continued)

Standard ID	A2	B2	C2	D2	E2
AccuStandard ID	S-4687-A	S-4687-B	S-4687-C	S-4687-D	S-4687-E
136		181			
148		192			
151		197			
144		199/201			
143		203			
142					
133					
161					
153					
130					
129					
166					
159					
167					
156					
179					
176					
178					
175					
183					
177					
171					
172					
191					
170					
190					
201/200					
204					
200/199					
198					
196					
195					
194					
207					
Total # of congeners	83	54	29	15	28

Table 4. Window defining congeners for SPB-Octyl and DB-1 columns

# Chlorines	First Eluter	Last Eluter	Labeled Reference	First eluter RT (min)	First eluter RRT	Last eluter RT (min)	Last eluter RRT
SPB-Octyl							
1	1	3	3	13.77	0.841	16.38	1.001
2	4	15	15	16.78	0.721	23.21	1.001
3	19	37	28	20.38	0.759	31.31	1.165
4	54	77	52	23.92	0.831	39.12	1.358
5	104	126	101	29.88	0.825	46.03	1.271
6	155	169	138	35.80	0.799	52.63	1.175
7	188	189	178	41.97	0.929	55.18	1.222
8	202	205	194	47.58	0.829	57.87	1.009
9	208	206	208	54.58	1.001	59.72	1.094
10	209		209		1.001		1.001
DB-1							
1	1	3	3	9.28	0.886	10.48	1.001
2	4	15	15	11.13	0.759	14.67	1.001
3	19	37	28	13.52	0.799	20.05	1.185
4	54	77	52	16.03	0.851	26.12	1.386
5	104	126	101	19.75	0.817	31.82	1.316
6	155	169	138	23.72	0.757	37.32	1.191
7	188	189	178	29.37	0.911	39.85	1.236
8	202	205	194	34.93	0.826	42.73	1.011
9	208	206	208	41.05	1.001	44.87	1.093
10	209		209	46.92	1.001		

Table 5a. GC conditions for SPB Octyl column

Column: 30m 0.25mm id 0.25 μ m film SPB-Octyl capillary column, (Supelco),

Injector: Split/splitless, at 270 °C, linear rate 37 cm/sec at 200 °C, (typical head pressure range 100 to 140 kPa), Septum purge 1.5 mL/min, total flow injector 50 mL/min

Injection: 1.0 μ L (CTC A200S auto sampler), in splitless mode, purge resumed after 2 minutes

Program: 75 °C for 2 min, 15 °C/min to 150°, 2.5 °C/min to 290 °C, hold for 1 min. Run time 64 min, PCB 209 elutes at approximately 61 minutes.

MS interface: Transfer lines 270 °C, column inserted directly into ion source.

Table 5b GC conditions for DB-1 column

Column: 30m 0.25mm i.d. 0.25 μ m film DB-1 capillary column, (J and W Scientific),

Injector: Split/splitless, at 270 °C, linear rate 40 cm/sec at 200 °C, (typical head pressure 85-100 kPa)

Injection: 1.0 μ L (CTC A200S auto sampler), in splitless mode, purge resumed after 2 minute

Program: 75 °C for 2 min, 15 °C/min to 150°, 2.5 °C/min to 270°C, hold for 7 min. Run time 61 min, PCB 209 elutes at approximately 48 minutes.

MS interface: Transfer lines 295 °C, column inserted directly into ion source.

Table 6a. Six function scan descriptor for SPB-Octyl column for 1668 full congener analysis

Function	Mass	m/z type	Ion formula	Substance
Fn-1	188.0393	M	12C12 H9 35Cl	Cl-1 PCB
Cl-1	190.0363	M+2	12C12 H9 37Cl	Cl-1 PCB
	200.0795	M	13C12 H9 35Cl	Cl-1 PCB
	202.0766	M+2	13C12 H9 37Cl	Cl-1 PCB
	218.9856	lock	C4 F9	PFK
Fn-2	222.0003	M	12C12 H8 35Cl2	Cl-2 PCB
Cl-2,3	223.9974	M+2	12C12 H8 35Cl 37 Cl	Cl-2 PCB
	225.9944	M+4	12C12 H8 37Cl2	Cl-2 PCB
	234.0406	M	13C12 H8 35Cl2	Cl-2 PCB
	236.0376	M+2	13C12 H8 35Cl 37 Cl	Cl-2 PCB
	242.9856	lock	C6 F9	PFK
	255.9613	M	12C12 H7 35Cl3	Cl-3 PCB
	257.9584	M+2	12C12 H7 35Cl2 37Cl	Cl-3 PCB
Fn-3	255.9613	M	12C12 H7 35Cl3	Cl-3 PCB
Cl-3,4,5	257.9584	M+2	12C12 H7 35Cl2 37Cl	Cl-3 PCB
	259.9554	M+4	12C12 H7 35Cl 37Cl2	Cl-3 PCB
	268.0016	M	13C12 H7 35Cl3	Cl-3 PCB
	269.9986	M+2	13C12 H7 35Cl2 37Cl	Cl-3 PCB
	280.9825	lock	C6 F11	PFK
	289.9224	M	12C12 H6 35Cl4	Cl-4 PCB
	291.9194	M+2	12C12 H6 35Cl3 37Cl	Cl-4 PCB
	293.9165	M+4	12C12 H6 35Cl2 37Cl2	Cl-4 PCB
	301.9626	M	13C12 H6 35Cl4	Cl-4 PCB
	303.9597	M+2	13C12 H6 35Cl3 37Cl	Cl-4 PCB
	323.8834	M	12C12 H5 35Cl5	Cl-5 PCB
	325.8804	M+2	12C12 H5 35Cl4 37Cl	Cl-5 PCB
	327.8775	M+4	12C12 H5 35Cl3 37Cl2	Cl-5 PCB
	337.9207	M+2	13C12 H5 35Cl4 37Cl	Cl-5 PCB
	339.9178	M+4	13C12 H5 35Cl3 37Cl2	Cl-5 PCB
Fn-4	289.9224	M	12C12 H6 35Cl4	Cl-4 PCB
Cl-4,5,6	291.9194	M+2	12C12 H6 35Cl3 37Cl	Cl-4 PCB
	293.9165	M+4	12C12 H6 35Cl2 37Cl2	Cl-4 PCB
	301.9626	M+2	13C12 H6 35Cl3 37Cl	Cl-4 PCB
	303.9597	M+4	13C12 H6 35Cl2 37Cl2	Cl-4 PCB
	323.8834	M	12C12 H5 35Cl5	Cl-5 PCB
	325.8804	M+2	12C12 H5 35Cl4 37Cl	Cl-5 PCB
	327.8775	M+4	12C12 H5 35Cl3 37Cl2	Cl-5 PCB

Table 6a (continued)

Function	Mass	m/z type	Ion formula	Substance	
Fn-4 (cont)	330.9792	lock	C7 F15	PFK	
	337.9207	M+2	13C12 H5 35Cl4 37Cl	Cl-5 PCB	13C12
	339.9178	M+4	13C12 H5 35Cl3 37Cl2	Cl-5 PCB	13C12
	359.8415	M	13C12 H4 35Cl6	Cl-6 PCB	
	361.8385	M+2	13C12 H4 35Cl5 37Cl	Cl-6 PCB	
	363.8356	M+4	13C12 H4 35Cl4 37Cl2	Cl-6 PCB	
	371.8817	M+2	13C12 H4 35Cl5 37Cl	Cl-6 PCB	13C12
	373.8788	M+4	13C12 H4 35Cl4 37Cl2	Cl-6 PCB	13C12
Fn-5	323.8834	M	12C12 H5 35Cl5	Cl-5 PCB	
Cl-5,6,7	325.8804	M+2	12C12 H5 35Cl4 37Cl	Cl-5 PCB	
	327.8775	M+4	12C12 H5 35Cl3 37Cl2	Cl-5 PCB	
	337.9207	M+2	13C12 H5 35Cl4 37Cl	Cl-5 PCB	13C12
	339.9178	M+4	13C12 H5 35Cl3 37Cl2	Cl-5 PCB	13C12
	354.9792	lock	C9 F13	PFK	
	359.8415	M+2	12C12 H4 35Cl5 37Cl	Cl-6 PCB	
	361.8385	M+4	12C12 H4 35Cl4 37Cl2	Cl-6 PCB	
	363.8356	M+6	12C12 H4 35Cl3 37Cl3	Cl-6 PCB	
	371.8817	M+2	13C12 H4 35Cl5 37Cl	Cl-6 PCB	13C12
	373.8788	M+4	13C12 H4 35Cl4 37Cl2	Cl-6 PCB	13C12
	393.8025	M+2	12C12 H3 35Cl6 37Cl	Cl-7 PCB	
	395.7995	M+4	12C12 H3 35Cl5 37Cl2	Cl-7 PCB	
	397.7966	M+6	12C12 H3 35Cl4 37Cl3	Cl-7 PCB	
	405.8428	M+2	13C12 H3 35Cl6 37Cl	Cl-7 PCB	13C12
	407.8398	M+4	13C12 H3 35Cl5 37Cl2	Cl-7 PCB	13C12
	454.9728	QC	C11 F17	PFK	

Table 6a (continued)

Function	Mass	m/z type	Ion formula	Substance
Fn-6	393.8025	M+2	12C12 H3 35Cl6 37Cl	Cl-7 PCB
Cl-7,8,9,10	395.7995	M+4	12C12 H3 35Cl5 37Cl2	Cl-7 PCB
	397.7966	M+6	12C12 H3 35Cl4 37Cl3	Cl-7 PCB
	405.8428	M+2	13C12 H3 35Cl6 37Cl	Cl-7 PCB
	407.8398	M+4	13C12 H3 35Cl5 37Cl2	Cl-7 PCB
	427.7635	M+2	12C12 H2 35Cl7 37Cl	Cl-8 PCB
	429.7606	M+4	12C12 H2 35Cl6 37Cl2	Cl-8 PCB
	431.7576	M+6	12C12 H2 35Cl5 37Cl3	Cl-8 PCB
	439.8038	M+2	13C12 H2 35Cl7 37Cl	Cl-8 PCB
	441.8008	M+4	13C12 H2 35Cl6 37Cl2	Cl-8 PCB
	442.9728	QC	C10 F13	PFK
	454.9728	lock	C11 F13	PFK
	461.7246	M+2	12C12 H1 35Cl8 37Cl	Cl-9 PCB
	463.7216	M+4	12C12 H1 35Cl7 37Cl2	Cl-9 PCB
	465.7187	M+6	12C12 H1 35Cl6 37Cl3	Cl-9 PCB
	473.7648	M+2	13C12 H1 35Cl8 37Cl	Cl-9 PCB
	475.7619	M+4	13C12 H1 35Cl7 37Cl2	Cl-9 PCB
	497.6826	M+4	12C12 35Cl8 37Cl2	Cl-10 PCB
	499.6797	M+6	12C12 35Cl7 37Cl3	Cl-10 PCB
	501.6767	M+8	12C12 35Cl6 37Cl4	Cl-10 PCB
	511.7199	M+4	13C12 35Cl9 37Cl	Cl-10 PCB
	513.7170	M+6	13C12 35Cl7 37Cl3	Cl-10 PCB
				13C12
				13C12

1. Isotopic masses used for accurate mass calculation

1 H	1.0078
12 C	12.0000
13 C	13.0034
35 Cl	34.9689
37 Cl	36.9659
19 F	18.9984

Table 6b. Six function scan descriptor for DB-1 column for 1668 full congener confirmation analysis

Function	Mass	m/z type	Ion formula	Substance
Fn-1	188.0393	M	12C12 H9 35Cl	Cl-1 PCB
Cl-1	190.0363	M+2	12C12 H9 37Cl	Cl-1 PCB
	200.0795	M	13C12 H9 35Cl	Cl-1 PCB
	202.0766	M+2	13C12 H9 37Cl	Cl-1 PCB
	218.9856	lock	C4 F9	PFK
Fn-2	222.0003	M	12C12 H8 35Cl2	Cl-2 PCB
Cl-2,3	223.9974	M+2	12C12 H8 35Cl 37 Cl	Cl-2 PCB
	225.9944	M+4	12C12 H8 37Cl2	Cl-2 PCB
	234.0406	M	13C12 H8 35Cl2	Cl-2 PCB
	236.0376	M+2	13C12 H8 35Cl 37 Cl	Cl-2 PCB
	242.9856	lock	C6 F9	PFK
	255.9613	M	12C12 H7 35Cl3	Cl-3 PCB
	257.9584	M+2	12C12 H7 35Cl2 37Cl	Cl-3 PCB
Fn-3	255.9613	M	12C12 H7 35Cl3	Cl-3 PCB
Cl-3,4,5	257.9584	M+2	12C12 H7 35Cl2 37Cl	Cl-3 PCB
	259.9554	M+4	12C12 H7 35Cl 37Cl2	Cl-3 PCB
	268.0016	M	13C12 H7 35Cl3	Cl-3 PCB
	269.9986	M+2	13C12 H7 35Cl2 37Cl	Cl-3 PCB
	280.9825	lock	C6 F11	PFK
	289.9224	M	12C12 H6 35Cl4	Cl-4 PCB
	291.9194	M+2	12C12 H6 35Cl3 37Cl	Cl-4 PCB
	293.9165	M+4	12C12 H6 35Cl2 37Cl2	Cl-4 PCB
	301.9626	M	13C12 H6 35Cl4	Cl-4 PCB
	303.9597	M+2	13C12 H6 35Cl3 37Cl	Cl-4 PCB
	323.8834	M	12C12 H5 35Cl5	Cl-5 PCB
	325.8804	M+2	12C12 H5 35Cl4 37Cl	Cl-5 PCB
	327.8775	M+4	12C12 H5 35Cl3 37Cl2	Cl-5 PCB
	337.9207	M+2	13C12 H5 35Cl4 37Cl	Cl-5 PCB
	339.9178	M+4	13C12 H5 35Cl3 37Cl2	Cl-5 PCB
Fn-4	289.9224	M	12C12 H6 35Cl4	Cl-4 PCB
Cl-4,5,6	291.9194	M+2	12C12 H6 35Cl3 37Cl	Cl-4 PCB
	293.9165	M+4	12C12 H6 35Cl2 37Cl2	Cl-4 PCB
	301.9626	M+2	13C12 H6 35Cl3 37Cl	Cl-4 PCB
	303.9597	M+4	13C12 H6 35Cl2 37Cl2	Cl-4 PCB
	323.8834	M	12C12 H5 35Cl5	Cl-5 PCB
	325.8804	M+2	12C12 H5 35Cl4 37Cl	Cl-5 PCB

Table 6b. (continued)

Function	Mass	m/z type	Ion formula	Substance	
	327.8775	M+4	12C12 H5 35Cl3 37Cl2	Cl-5 PCB	
Fn-4 (cont)	330.9792	lock	C7 F15	PFK	
	337.9207	M+2	13C12 H5 35Cl4 37Cl	Cl-5 PCB	13C12
	339.9178	M+4	13C12 H5 35Cl3 37Cl2	Cl-5 PCB	13C12
	359.8415	M	13C12 H4 35Cl6	Cl-6 PCB	
	361.8385	M+2	13C12 H4 35Cl5 37Cl	Cl-6 PCB	
	363.8356	M+4	13C12 H4 35Cl4 37Cl2	Cl-6 PCB	
	371.8817	M+2	13C12 H4 35Cl5 37Cl	Cl-6 PCB	13C12
	373.8788	M+4	13C12 H4 35Cl4 37Cl2	Cl-6 PCB	13C12
Fn-5	323.8834	M	12C12 H5 35Cl5	Cl-5 PCB	
Cl-5,6,7,8	325.8804	M+2	12C12 H5 35Cl4 37Cl	Cl-5 PCB	
	327.8775	M+4	12C12 H5 35Cl3 37Cl2	Cl-5 PCB	
	337.9207	M+2	13C12 H5 35Cl4 37Cl	Cl-5 PCB	13C12
	339.9178	M+4	13C12 H5 35Cl3 37Cl2	Cl-5 PCB	13C12
	354.9792	lock	C9 F13	PFK	
	359.8415	M+2	12C12 H4 35Cl5 37Cl	Cl-6 PCB	
	361.8385	M+4	12C12 H4 35Cl4 37Cl2	Cl-6 PCB	
	363.8356	M+6	12C12 H4 35Cl3 37Cl3	Cl-6 PCB	
	371.8817	M+2	13C12 H4 35Cl5 37Cl	Cl-6 PCB	13C12
	373.8788	M+4	13C12 H4 35Cl4 37Cl2	Cl-6 PCB	13C12
	393.8025	M+2	12C12 H3 35Cl6 37Cl	Cl-7 PCB	
	395.7995	M+4	12C12 H3 35Cl5 37Cl2	Cl-7 PCB	
	397.7966	M+6	12C12 H3 35Cl4 37Cl3	Cl-7 PCB	
	405.8428	M+2	13C12 H3 35Cl6 37Cl	Cl-7 PCB	13C12
	407.8398	M+4	13C12 H3 35Cl5 37Cl2	Cl-7 PCB	13C12
	427.7635	M+2	12C12 H2 35Cl7 37Cl	Cl-8 PCB	
	429.7606	M+4	12C12 H2 35Cl6 37Cl2	Cl-8 PCB	
	431.7576	M+6	12C12 H2 35Cl5 37Cl3	Cl-8 PCB	
	439.8038	M+2	13C12 H2 35Cl7 37Cl	Cl-8 PCB	13C12
	441.8008	M+4	13C12 H2 35Cl6 37Cl2	Cl-8 PCB	13C12
	454.9728	QC	C11 F17	PFK	

Table 6b. (continued)

Function	Mass	m/z type	Ion formula	Substance
Fn-6	427.7635	M+2	12C12 H2 35Cl7 37Cl	Cl-8 PCB
Cl-8,9,10	429.7606	M+4	12C12 H2 35Cl6 37Cl2	Cl-8 PCB
	431.7576	M+6	12C12 H2 35Cl5 37Cl3	Cl-8 PCB
	439.8038	M+2	13C12 H2 35Cl7 37Cl	Cl-8 PCB
	441.8008	M+4	13C12 H2 35Cl6 37Cl2	Cl-8 PCB
	442.9728	QC	C10 F13	PFK
	454.9728	lock	C11 F13	PFK
	461.7246	M+2	12C12 H1 35Cl8 37Cl	Cl-9 PCB
	463.7216	M+4	12C12 H1 35Cl7 37Cl2	Cl-9 PCB
	465.7187	M+6	12C12 H1 35Cl6 37Cl3	Cl-9 PCB
	473.7648	M+2	13C12 H1 35Cl8 37Cl	Cl-9 PCB
	475.7619	M+4	13C12 H1 35Cl7 37Cl2	Cl-9 PCB
	497.6826	M+4	12C12 35Cl8 37Cl2	Cl-10 PCB
	499.6797	M+6	12C12 35Cl7 37Cl3	Cl-10 PCB
	501.6767	M+8	12C12 35Cl6 37Cl4	Cl-10 PCB
	511.7199	M+4	13C12 35Cl9 37Cl	Cl-10 PCB
	513.7170	M+6	13C12 35Cl7 37Cl3	Cl-10 PCB
				13C12
				13C12

1. Isotopic masses used for accurate mass calculation

1 H	1.0078
12 C	12.0000
13 C	13.0034
35 Cl	34.9689
37 Cl	36.9659
19 F	18.9984

Table 6c. Summary of distribution of homologue groups acquired within the six function Octyl and DB-1 scan descriptors.

Function # in Scan Descriptor	Octyl Column	DB-1 Column
	Homologue group acquired (LOC)	Homologue group acquired (LOC)
1	1	1
2	2,3	2,3
3	3,4,5	3,4,5
4	4,5,6	4,5,6
5	5,6,7	5,6,7,8
6	7,8,9,10	8,9,10

Table 7a. Analyte table for targeting Octyl data with OpusQuan

Ent	Type	Name	Method	Std	Amo ng	1.00	2.00	RT	Win. sec	Std.	Fn	m1	m2	m1/m2	Tol.
Part 1. Analyte table 1668XA-Octyl-C for Cl1 to Cl4															
1	Unk	CL1-PCB-1	rel_int	66	50	y	n	13:38	6	66	1	188.04	190.04	3.13	0.15
2	Unk	CL1-PCB-2	rel_int	66	50	y	n	16:02	6	66	1	188.04	190.04	3.13	0.15
3	Unk	CL1-PCB-3	rel_int	66	50	y	n	16:15	6	66	1	188.04	190.04	3.13	0.15
4	Unk	CL2-PCB-4	rel_int	67	50	y	n	16:34	6	67	2	222	224	1.56	0.15
5	Unk	CL2-PCB-10	rel_int	67	50	y	n	16:46	6	67	2	222	224	1.56	0.15
6	Unk	CL2-PCB-9	rel_int	67	50	y	n	18:51	6	67	2	222	224	1.56	0.15
7	Unk	CL2-PCB-7	rel_int	67	50	y	n	19:02	6	67	2	222	224	1.56	0.15
8	Unk	CL2-PCB-6	rel_int	67	50	y	n	19:19	6	67	2	222	224	1.56	0.15
9	Unk	CL2-PCB-5	rel_int	67	50	y	n	19:41	6	67	2	222	224	1.56	0.15
10	Unk	CL2-PCB-8	rel_int	67	50	y	n	19:49	6	67	2	222	224	1.56	0.15
11	Unk	CL2-PCB-14	rel_int	67	50	y	n	21:39	6	67	2	222	224	1.56	0.15
12	Unk	CL2-PCB-11	rel_int	67	50	y	n	22:38	6	67	2	222	224	1.56	0.15
13	Unk	CL2-PCB-12/13	rel_int	67	100	y	n	22:59	10	67	2	222	224	1.56	0.15
14	Unk	CL2-PCB-15	rel_int	67	50	y	n	23:19	6	67	2	222	224	1.56	0.15
15	Unk	CL3-PCB-19	rel_int	68	50	y	n	20:12	6	68	2	255.96	257.96	1.04	0.15
16	Unk	CL3-PCB-30/18	rel_int	68	100	y	n	22:14	10	68	2	255.96	257.96	1.04	0.15
17	Unk	CL3-PCB-17	rel_int	68	50	y	n	22:46	6	68	2	255.96	257.96	1.04	0.15
18	Unk	CL3-PCB-27	rel_int	68	50	y	n	23:00	6	68	2	255.96	257.96	1.04	0.15
19	Unk	CL3-PCB-24	rel_int	68	50	y	n	23:08	6	68	2	255.96	257.96	1.04	0.15
20	Unk	CL3-PCB-16	rel_int	68	50	y	n	23:18	6	68	2	255.96	257.96	1.04	0.15
21	Unk	CL3-PCB-32	rel_int	68	50	y	n	23:51	6	68	3	255.96	257.96	1.04	0.15
22	Unk	CL3-PCB-34	rel_int	68	50	y	n	25:14	6	68	3	255.96	257.96	1.04	0.15
23	Unk	CL3-PCB-23	rel_int	68	50	y	n	25:23	6	68	3	255.96	257.96	1.04	0.15
24	Unk	CL3-PCB-26/29	rel_int	68	100	y	n	25:46	10	68	3	255.96	257.96	1.04	0.15
25	Unk	CL3-PCB-25	rel_int	68	50	y	n	26:00	6	68	3	255.96	257.96	1.04	0.15
26	Unk	CL3-PCB-31	rel_int	68	50	y	n	26:21	6	68	3	255.96	257.96	1.04	0.15
27	Unk	CL3-PCB-28/20	rel_int	68	100	y	n	26:43	10	68	3	255.96	257.96	1.04	0.15
28	Unk	CL3-PCB-21/33	rel_int	68	100	y	n	26:53	10	68	3	255.96	257.96	1.04	0.15
29	Unk	CL3-PCB-22	rel_int	68	50	y	n	27:24	6	68	3	255.96	257.96	1.04	0.15
30	Unk	CL3-PCB-36	rel_int	68	50	y	n	29:05	6	68	3	255.96	257.96	1.04	0.15
31	Unk	CL3-PCB-39	rel_int	68	50	y	n	29:28	6	68	3	255.96	257.96	1.04	0.15
32	Unk	CL3-PCB-38	rel_int	68	50	y	n	30:08	6	68	3	255.96	257.96	1.04	0.15
33	Unk	CL3-PCB-35	rel_int	68	50	y	n	30:38	6	68	3	255.96	257.96	1.04	0.15
34	Unk	CL3-PCB-37	rel_int	68	50	y	n	31:05	6	68	3	255.96	257.96	1.04	0.15
35	Unk	CL4-PCB-54	rel_int	69	100	y	n	23:42	6	69	3	289.92	291.92	0.77	0.15
36	Unk	CL4-PCB-50/53	rel_int	69	200	y	n	26:05	10	69	3	289.92	291.92	0.77	0.15
37	Unk	CL4-PCB-45/51	rel_int	69	200	y	n	26:50	10	69	3	289.92	291.92	0.77	0.15
38	Unk	CL4-PCB-46	rel_int	69	100	y	n	27:10	6	69	3	289.92	291.92	0.77	0.15
39	Unk	CL4-PCB-52	rel_int	69	100	y	n	28:41	6	69	3	289.92	291.92	0.77	0.15
40	Unk	CL4-PCB-73	rel_int	69	100	y	n	28:50	6	69	3	289.92	291.92	0.77	0.15

Table 7a. (continued)

Ent	Type	Name	Method	Std	Amo	1.00	2.00	RT	Win.	Std.	Fn	m1	m2	m1/m2	Tol.
				ng					sec						
41	Unk	CL4-PCB-43	rel_int	69	100	y	n	28:55	6	69	3	289.92	291.92	0.77	0.15
42	Unk	CL4-PCB-69/49	rel_int	69	200	y	n	29:10	10	69	3	289.92	291.92	0.77	0.15
43	Unk	CL4-PCB-48	rel_int	69	100	y	n	29:32	6	69	3	289.92	291.92	0.77	0.15
44	Unk	CL4-PCB-44/47/65	rel_int	69	300	y	n	29:48	10	69	3	289.92	291.92	0.77	0.15
45	Unk	CL4-PCB-59/62/75	rel_int	69	300	y	n	30:09	10	69	3	289.92	291.92	0.77	0.15
46	Unk	CL4-PCB-42	rel_int	69	100	y	n	30:22	6	69	3	289.92	291.92	0.77	0.15
47	Unk	CL4-PCB-41	rel_int	69	100	y	n	30:48	6	69	3	289.92	291.92	0.77	0.15
48	Unk	CL4-PCB-40/71	rel_int	69	200	y	n	30:55	10	69	3	289.92	291.92	0.77	0.15
49	Unk	CL4-PCB-64	rel_int	69	100	y	n	31:09	6	69	3	289.92	291.92	0.77	0.15
50	Unk	CL4-PCB-72	rel_int	69	100	y	n	32:00	6	69	4	289.92	291.92	0.77	0.15
51	Unk	CL4-PCB-68	rel_int	69	100	y	n	32:19	6	69	4	289.92	291.92	0.77	0.15
52	Unk	CL4-PCB-57	rel_int	69	100	y	n	32:47	6	69	4	289.92	291.92	0.77	0.15
53	Unk	CL4-PCB-58	rel_int	69	100	y	n	33:03	6	69	4	289.92	291.92	0.77	0.15
54	Unk	CL4-PCB-67	rel_int	69	100	y	n	33:14	6	69	4	289.92	291.92	0.77	0.15
55	Unk	CL4-PCB-63	rel_int	69	100	y	n	33:31	6	69	4	289.92	291.92	0.77	0.15
56	Unk	CL4-PCB-61/70/74/76	rel_int	69	400	y	n	33:53	12	69	4	289.92	291.92	0.77	0.15
57	Unk	CL4-PCB-66	rel_int	69	100	y	n	34:14	6	69	4	289.92	291.92	0.77	0.15
58	Unk	CL4-PCB-55	rel_int	69	100	y	n	34:26	6	69	4	289.92	291.92	0.77	0.15
59	Unk	CL4-PCB-56	rel_int	69	100	y	n	34:57	6	69	4	289.92	291.92	0.77	0.15
60	Unk	CL4-PCB-60	rel_int	69	100	y	n	35:13	6	69	4	289.92	291.92	0.77	0.15
61	Unk	CL4-PCB-80	rel_int	69	100	y	n	35:35	6	69	4	289.92	291.92	0.77	0.15
62	Unk	CL4-PCB-79	rel_int	69	100	y	n	37:16	6	69	4	289.92	291.92	0.77	0.15
63	Unk	CL4-PCB-78	rel_int	69	100	y	n	37:53	6	69	4	289.92	291.92	0.77	0.15
64	Unk	CL4-PCB-81	rel_int	69	100	y	n	38:21	6	69	4	289.92	291.92	0.77	0.15
65	Unk	CL4-PCB-77	rel_int	69	100	y	n	38:58	6	69	4	289.92	291.92	0.77	0.15
66	IS	13C-CL1-PCB-3	rel_int	70	100	n	y	16:14	10	70	1	200.08	202.08	3.13	0.15
67	IS	13C-CL2-PCB-15	rel_int	70	100	n	y	23:18	10	70	2	234.04	236.04	1.56	0.15
68	IS	13C-CL3-PCB-28	rel_int	70	100	n	y	26:39	10	70	3	268	270	1.04	0.15
69	IS	13C-CL4-PCB-77	rel_int	70	100	n	y	38:57	10	70	4	301.96	303.96	0.77	0.15
70	RS/RT	13C-CL4-PCB-52	abs_int	500	n	y		28:40	25		3	301.96	303.96	0.77	0.15
71	C/Up	13C-CL4-PCB-81	rel_int	70	50	y	y	38:20	10	70	4	301.96	303.96	0.77	0.15

Part 2. Analyte table 1668XB-Octyl-C for Cl 5s

1	Unk	CL5-PCB-104	rel_int	32	100	y	n	29:44	6	32	3	325.88	327.88	1.55	0.15
2	Unk	CL5-PCB-96	rel_int	32	100	y	n	30:11	6	32	3	325.88	327.88	1.55	0.15
3	Unk	CL5-PCB-103	rel_int	32	100	y	n	32:13	6	32	4	325.88	327.88	1.55	0.15
4	Unk	CL5-PCB-94	rel_int	32	100	y	n	32:28	6	32	4	325.88	327.88	1.55	0.15
5	Unk	CL5-PCB-95	rel_int	32	100	y	n	32:57	6	32	4	325.88	327.88	1.55	0.15
6	Unk	CL5-PCB-100/93	rel_int	32	200	y	n	33:10	10	32	4	325.88	327.88	1.55	0.15
7	Unk	CL5-PCB-102/98	rel_int	32	200	y	n	33:19	12	32	4	325.88	327.88	1.55	0.15
8	Unk	CL5-PCB-88/91	rel_int	32	200	y	n	33:46	12	32	4	325.88	327.88	1.55	0.15

Table 7a. (continued)

Ent	Type	Name	Method	Std	Amo ng	1.00	2.00	RT	Win. sec	Std.	Fn	m1	m2	m1/m2	Tol.
9	Unk	CL5-PCB-84	rel_int	32	100	y	n	34:09	6	32	4	325.88	327.88	1.55	0.15
10	Unk	CL5-PCB-89	rel_int	32	100	y	n	34:40	6	32	4	325.88	327.88	1.55	0.15
11	Unk	CL5-PCB-121	rel_int	32	100	y	n	35:02	6	32	4	325.88	327.88	1.55	0.15
12	Unk	CL5-PCB-92	rel_int	32	100	y	n	35:28	6	32	4	325.88	327.88	1.55	0.15
13	Unk	CL5-PCB-113/90/101	rel_int	32	300	y	n	36:05	10	32	4	325.88	327.88	1.55	0.15
14	Unk	CL5-PCB-83/99	rel_int	32	200	y	n	36:37	12	32	4	325.88	327.88	1.55	0.15
15	Unk	CL5-PCB-112	rel_int	32	100	y	n	36:51	6	32	4	325.88	327.88	1.55	0.15
16	Unk	PCB-108/119/86/97/125/87	rel_int	32	600	y	n	37:16	16	32	4	325.88	327.88	1.55	0.15
17	Unk	CL5-PCB-117/116/85	rel_int	32	300	y	n	38:00	12	32	4	325.88	327.88	1.55	0.15
18	Unk	CL5-PCB-110/115	rel_int	32	200	y	n	38:14	10	32	4	325.88	327.88	1.55	0.15
19	Unk	CL5-PCB-82	rel_int	32	100	y	n	38:36	6	32	4	325.88	327.88	1.55	0.15
20	Unk	CL5-PCB-111	rel_int	32	100	y	n	38:56	6	32	4	325.88	327.88	1.55	0.15
21	Unk	CL5-PCB-120	rel_int	32	100	y	n	39:26	6	32	4	325.88	327.88	1.55	0.15
22	Unk	CL5-PCB-107/124	rel_int	32	200	y	n	40:41	10	32	5	325.88	327.88	1.55	0.15
23	Unk	CL5-PCB-109	rel_int	32	100	y	n	40:56	6	32	5	325.88	327.88	1.55	0.15
24	Unk	CL5-PCB-123	rel_int	32	100	y	n	41:03	6	32	5	325.88	327.88	1.55	0.15
25	Unk	CL5-PCB-106	rel_int	32	100	y	n	41:13	6	32	5	325.88	327.88	1.55	0.15
26	Unk	CL5-PCB-118	rel_int	32	100	y	n	41:23	6	32	5	325.88	327.88	1.55	0.15
27	Unk	CL5-PCB-122	rel_int	32	100	y	n	41:47	6	32	5	325.88	327.88	1.55	0.15
28	Unk	CL5-PCB-114	rel_int	32	100	y	n	42:00	6	32	5	325.88	327.88	1.55	0.15
29	Unk	CL5-PCB-105	rel_int	33	100	y	n	42:42	6	33	5	325.88	327.88	1.55	0.15
30	Unk	CL5-PCB-127	rel_int	34	100	y	n	44:14	6	34	5	325.88	327.88	1.55	0.15
31	Unk	CL5-PCB-126	rel_int	34	100	y	n	45:59	6	34	5	325.88	327.88	1.55	0.15
32	IS	13C-CL5-PCB-118	rel_int	35	100	n	y	41:22	10	35	5	335.92	337.92	0.63	0.15
33	IS	13C-CL5-PCB-105	rel_int	35	100	n	y	42:41	10	35	5	335.92	337.92	0.63	0.15
34	IS	13C-CL5-PCB-126	rel_int	35	100	n	y	45:58	10	35	5	335.92	337.92	0.63	0.15
35	RS/RT	13C-CL5-PCB-101	abs_int	500	n	y		36:04	25	4	335.92	337.92	0.63	0.15	
36	C/Up	13C-CL5-PCB-111	rel_int	35	250	y	y	38:55	10	35	4	335.92	337.92	0.63	0.15

Part 3. Analyte table 1668XC-Octyl-C for Cl6s

1	Unk	CL6-PCB-155	rel_int	33	100	y	n	35:50	6	33	4	359.84	361.84	1.24	0.15
2	Unk	CL6-PCB-152	rel_int	33	100	y	n	36:05	6	33	4	359.84	361.84	1.24	0.15
3	Unk	CL6-PCB-150	rel_int	33	100	y	n	36:16	6	33	4	359.84	361.84	1.24	0.15
4	Unk	CL6-PCB-136	rel_int	33	100	y	n	36:40	6	33	4	359.84	361.84	1.24	0.15
5	Unk	CL6-PCB-145	rel_int	33	100	y	n	36:59	6	33	4	359.84	361.84	1.24	0.15
6	Unk	CL6-PCB-148	rel_int	33	100	y	n	38:32	6	33	4	359.84	361.84	1.24	0.15
7	Unk	CL6-PCB-151/135	rel_int	33	200	y	n	39:13	10	33	4	359.84	361.84	1.24	0.15
8	Unk	CL6-PCB-154	rel_int	33	100	y	n	39:26	6	33	4	359.84	361.84	1.24	0.15
9	Unk	CL6-PCB-144	rel_int	33	100	y	n	39:48	6	33	4	359.84	361.84	1.24	0.15
10	Unk	CL6-PCB-147/149	rel_int	33	200	y	n	40:12	10	33	5	359.84	361.84	1.24	0.15
11	Unk	CL6-PCB-134/143	rel_int	33	200	y	n	40:28	10	33	5	359.84	361.84	1.24	0.15

Table 7a. (continued)

Ent	Type	Name	Method	Std	Amo	1.00	2.00	RT	Win.	Std.	Fn	m1	m2	m1/m2	Tol.
				ng				sec							
12	Unk	CL6-PCB-139/140	rel_int	33	200	y	n	40:49	10	33	5	359.84	361.84	1.24	0.15
13	Unk	CL6-PCB-131	rel_int	33	100	y	n	41:05	6	33	5	359.84	361.84	1.24	0.15
14	Unk	CL6-PCB-142	rel_int	33	100	y	n	41:14	6	33	5	359.84	361.84	1.24	0.15
15	Unk	CL6-PCB-132	rel_int	33	100	y	n	41:34	6	33	5	359.84	361.84	1.24	0.15
16	Unk	CL6-PCB-133	rel_int	33	100	y	n	42:02	6	33	5	359.84	361.84	1.24	0.15
17	Unk	CL6-PCB-165	rel_int	33	100	y	n	42:27	6	33	5	359.84	361.84	1.24	0.15
18	Unk	CL6-PCB-146	rel_int	33	100	y	n	42:43	6	33	5	359.84	361.84	1.24	0.15
19	Unk	CL6-PCB-161	rel_int	33	100	y	n	42:51	6	33	5	359.84	361.84	1.24	0.15
20	Unk	CL6-PCB-153/168	rel_int	33	200	y	n	43:24	10	33	5	359.84	361.84	1.24	0.15
21	Unk	CL6-PCB-141	rel_int	33	100	y	n	43:37	6	33	5	359.84	361.84	1.24	0.15
22	Unk	CL6-PCB-130	rel_int	33	100	y	n	44:03	6	33	5	359.84	361.84	1.24	0.15
23	Unk	CL6-PCB-137	rel_int	33	100	y	n	44:17	6	33	5	359.84	361.84	1.24	0.15
24	Unk	CL6-PCB-164	rel_int	33	100	y	n	44:24	6	33	5	359.84	361.84	1.24	0.15
25	Unk	CL6-PCB-138/163/129/160	rel_int	33	400	y	n	44:45	14	33	5	359.84	361.84	1.24	0.15
26	Unk	CL6-PCB-158	rel_int	33	100	y	n	45:09	6	33	5	359.84	361.84	1.24	0.15
27	Unk	CL6-PCB-128/166	rel_int	33	200	y	n	46:05	10	33	5	359.84	361.84	1.24	0.15
28	Unk	CL6-PCB-159	rel_int	33	100	y	n	47:06	6	33	5	359.84	361.84	1.24	0.15
29	Unk	CL6-PCB-162	rel_int	33	100	y	n	47:23	6	33	5	359.84	361.84	1.24	0.15
30	Unk	CL6-PCB-167	rel_int	33	100	y	n	47:53	6	33	5	359.84	361.84	1.24	0.15
31	Unk	CL6-PCB-156/157	rel_int	34	200	y	n	49:09	10	34	5	359.84	361.84	1.24	0.15
32	Unk	CL6-PCB-169	rel_int	35	100	y	n	52:34	6	35	5	359.84	361.84	1.24	0.15
33	IS	13C-CL6-PCB-167	rel_int	36	100	n	y	47:52	10	36	5	371.88	373.89	1.24	0.15
34	IS	13C-CL6-PCB-156/157	rel_int	36	200	n	y	49:06	10	36	5	371.88	373.88	1.24	0.15
35	IS	13C-CL6-PCB-169	rel_int	36	100	n	y	52:33	10	36	5	371.88	373.89	1.24	0.15
36	RS/RT	13C-CL6-PCB-138	abs_int	500	n	y		44:42	25	5	371.88	373.88	1.24	0.15	

Part 4. Analyte table 1668XD-Octyl-C for C7 to Cl 10

1	Unk	CL7-PCB-188	rel_int	38	100	y	n	41:56	6	38	5	393.80	395.80	1.05	0.15
2	Unk	CL7-PCB-179	rel_int	38	100	y	n	42:21	6	38	5	393.80	395.80	1.05	0.15
3	Unk	CL7-PCB-184	rel_int	38	100	y	n	42:52	6	38	5	393.80	395.80	1.05	0.15
4	Unk	CL7-PCB-176	rel_int	38	100	y	n	43:17	6	38	5	393.80	395.80	1.05	0.15
5	Unk	CL7-PCB-186	rel_int	38	100	y	n	43:47	6	38	5	393.80	395.80	1.05	0.15
6	Unk	CL7-PCB-178	rel_int	38	100	y	n	45:11	6	38	5	393.80	395.80	1.05	0.15
7	Unk	CL7-PCB-175	rel_int	38	100	y	n	45:52	6	38	5	393.80	395.80	1.05	0.15
8	Unk	CL7-PCB-187	rel_int	38	100	y	n	46:08	6	38	5	393.80	395.80	1.05	0.15
9	Unk	CL7-PCB-182	rel_int	38	100	y	n	46:22	6	38	5	393.80	395.80	1.05	0.15
10	Unk	CL7-PCB-183	rel_int	38	100	y	n	46:47	6	38	5	393.80	395.80	1.05	0.15
11	Unk	CL7-PCB-185	rel_int	38	100	y	n	46:55	6	38	5	393.80	395.80	1.05	0.15
12	Unk	CL7-PCB-174	rel_int	38	100	y	n	47:05	6	38	5	393.80	395.80	1.05	0.15
13	Unk	CL7-PCB-177	rel_int	38	100	y	n	47:32	6	38	5	393.80	395.80	1.05	0.15
14	Unk	CL7-PCB-181	rel_int	38	100	y	n	47:58	6	38	5	393.80	395.80	1.05	0.15

Table 7a. (continued)

Ent	Type	Name	Method	Std	Amo	1.00	2.00	RT	Win. sec	Std.	Fn	m1	m2	m1/m2	Tol.
					ng										
15	Unk	CL7-PCB-171/173	rel_int	38	200	y	n	48:12	10	38	5	393.80	395.80	1.05	0.15
16	Unk	CL7-PCB-172	rel_int	38	100	y	n	49:54	6	38	5	393.80	395.80	1.05	0.15
17	Unk	CL7-PCB-192	rel_int	38	100	y	n	50:12	6	38	5	393.80	395.80	1.05	0.15
18	Unk	CL7-PCB-193/180	rel_int	38	200	y	n	50:34	10	38	5	393.80	395.80	1.05	0.15
19	Unk	CL7-PCB-191	rel_int	38	100	y	n	50:59	6	38	5	393.80	395.80	1.05	0.15
20	Unk	CL7-PCB-170	rel_int	38	100	y	n	51:59	6	38	5	393.80	395.80	1.05	0.15
21	Unk	CL7-PCB-190	rel_int	38	100	y	n	52:32	6	38	5	393.80	395.80	1.05	0.15
22	Unk	CL7-PCB-189	rel_int	39	100	y	n	55:14	6	39	6	393.80	395.80	1.05	0.15
23	Unk	CL8-PCB-202	rel_int	40	150	y	n	47:39	6	40	5	427.76	429.76	0.89	0.15
24	Unk	CL8-PCB-201	rel_int	40	150	y	n	48:38	6	40	5	427.76	429.76	0.89	0.15
25	Unk	CL8-PCB-204	rel_int	40	150	y	n	49:21	6	40	5	427.76	429.76	0.89	0.15
26	Unk	CL8-PCB-197	rel_int	40	150	y	n	49:35	6	40	5	427.76	429.76	0.89	0.15
27	Unk	CL8-PCB-200	rel_int	40	150	y	n	49:44	7	40	5	427.76	429.76	0.89	0.15
28	Unk	CL8-PCB-198/199	rel_int	40	300	y	n	52:39	10	40	5	427.76	429.76	0.89	0.15
29	Unk	CL8-PCB-196	rel_int	40	150	y	n	53:22	6	40	5	427.76	429.76	0.89	0.15
30	Unk	CL8-PCB-203	rel_int	40	150	y	n	53:34	6	40	5	427.76	429.76	0.89	0.15
31	Unk	CL8-PCB-195	rel_int	40	150	y	n	55:02	6	40	6	427.76	429.76	0.89	0.15
32	Unk	CL8-PCB-194	rel_int	40	150	y	n	57:28	6	40	6	427.76	429.76	0.89	0.15
33	Unk	CL8-PCB-205	rel_int	40	150	y	n	57:57	6	40	6	427.76	429.76	0.89	0.15
34	Unk	CL9-PCB-208	rel_int	41	150	y	n	54:44	6	41	6	461.72	463.72	0.78	0.15
35	Unk	CL9-PCB-207	rel_int	41	150	y	n	55:43	6	41	6	461.72	463.72	0.78	0.15
36	Unk	CL9-PCB-206	rel_int	41	150	y	n	59:48	7	41	6	461.72	463.72	0.78	0.15
37	Unk	CL10-PCB-209	rel_int	42	150	y	n	61:22	6	42	6	495.69	497.68	0.69	0.15
38	IS	13C-CL7-PCB-180	rel_int	43	100	n	y	50:35	10	43	5	405.80	407.84	1.05	0.15
39	IS	13C-CL7-PCB-189	rel_int	43	100	n	y	55:13	10	43	6	405.80	407.84	1.05	0.15
40	IS	13C-CL8-PCB-194	rel_int	43	100	n	y	57:27	10	43	6	439.80	441.80	0.89	0.15

Table 7b. Analyte table for targeting DB-1 data with OpusQuan

Ent	Type	Name	Method	Std	Amo ng	1	2	RT	Win. sec	Std.	Fn	m1	m2	m1/m2	Tol.
Part 1. Analyte table 1668XA-DB1-C for Cl1 to Cl4															
1	Unk	CL1-PCB-1	rel_int	62	50	y	n	09:41	6	62	1	188.04	190.04	3.13	0.15
2	Unk	CL1-PCB-2	rel_int	62	50	y	n	10:50	6	62	1	188.04	190.04	3.13	0.15
3	Unk	CL1-PCB-3	rel_int	62	50	y	n	10:57	6	62	1	188.04	190.04	3.13	0.15
4	Unk	CL2-PCB-4/10	rel_int	63	100	y	n	11:40	10	63	2	222	224	1.56	0.15
5	Unk	CL2-PCB-7/9	rel_int	63	100	y	n	12:41	10	63	2	222	224	1.56	0.15
6	Unk	CL2-PCB-6	rel_int	63	50	y	n	13:05	6	63	2	222	224	1.56	0.15
7	Unk	CL2-PCB-8/5	rel_int	63	100	y	n	13:20	10	63	2	222	224	1.56	0.15
8	Unk	CL2-PCB-14	rel_int	63	50	y	n	14:02	6	63	2	222	224	1.56	0.15
9	Unk	CL2-PCB-11	rel_int	63	50	y	n	14:50	6	63	2	222	224	1.56	0.15
10	Unk	CL2-PCB-13/12	rel_int	63	100	y	n	15:06	10	63	2	222	224	1.56	0.15
11	Unk	CL2-PCB-15	rel_int	63	50	y	n	15:18	6	63	2	222	224	1.56	0.15
12	Unk	CL3-PCB-19	rel_int	64	50	y	n	14:08	6	64	2	255.96	257.96	1.04	0.15
13	Unk	CL3-PCB-30	rel_int	64	50	y	n	14:44	6	64	2	255.96	257.96	1.04	0.15
14	Unk	CL3-PCB-18	rel_int	64	50	y	n	15:15	6	64	2	255.96	257.96	1.04	0.15
15	Unk	CL3-PCB-17	rel_int	64	50	y	n	15:23	6	64	2	255.96	257.96	1.04	0.15
16	Unk	CL3-PCB-24/27	rel_int	64	100	y	n	15:47	10	64	2	255.96	257.96	1.04	0.15
17	Unk	CL3-PCB-16/32	rel_int	64	100	y	n	16:10	12	64	2	255.96	257.96	1.04	0.15
18	Unk	CL3-PCB-34/23	rel_int	64	100	y	n	16:49	12	64	3	255.96	257.96	1.04	0.15
19	Unk	CL3-PCB-26	rel_int	64	50	y	n	17:12	6	64	3	255.96	257.96	1.04	0.15
20	Unk	CL3-PCB-29	rel_int	64	50	y	n	17:01	6	64	3	255.96	257.96	1.04	0.15
21	Unk	CL3-PCB-25	rel_int	64	50	y	n	17:18	6	64	3	255.96	257.96	1.04	0.15
22	Unk	CL3-PCB-31/28	rel_int	64	100	y	n	17:37	12	64	3	255.96	257.96	1.04	0.15
23	Unk	CL3-PCB-20/21/33	rel_int	64	150	y	n	18:07	10	64	3	255.96	257.96	1.04	0.15
24	Unk	CL3-PCB-22	rel_int	64	50	y	n	18:29	6	64	3	255.96	257.96	1.04	0.15
25	Unk	CL3-PCB-36	rel_int	64	50	y	n	19:02	6	64	3	255.96	257.96	1.04	0.15
26	Unk	CL3-PCB-39	rel_int	64	50	y	n	19:24	6	64	3	255.96	257.96	1.04	0.15
27	Unk	CL3-PCB-38	rel_int	64	50	y	n	20:01	6	64	3	255.96	257.96	1.04	0.15
28	Unk	CL3-PCB-35	rel_int	64	50	y	n	20:28	6	64	3	255.96	257.96	1.04	0.15
29	Unk	CL3-PCB-37	rel_int	64	50	y	n	20:50	6	64	3	255.96	257.96	1.04	0.15
30	Unk	CL4-PCB-54	rel_int	65	100	y	n	16:45	6	65	3	289.92	291.92	0.77	0.15
31	Unk	CL4-PCB-50	rel_int	65	100	y	n	17:41	6	65	3	289.92	291.92	0.77	0.15
32	Unk	CL4-PCB-53	rel_int	65	100	y	n	18:12	6	65	3	289.92	291.92	0.77	0.15
33	Unk	CL4-PCB-45	rel_int	65	100	y	n	18:48	6	65	3	289.92	291.92	0.77	0.15
34	Unk	CL4-PCB-51	rel_int	65	100	y	n	18:28	6	65	3	289.92	291.92	0.77	0.15
35	Unk	CL4-PCB-46	rel_int	65	100	y	n	19:12	6	65	3	289.92	291.92	0.77	0.15
36	Unk	CL4-PCB-73	rel_int	65	100	y	n	19:45	6	65	3	289.92	291.92	0.77	0.15
37	Unk	CL4-PCB-52/69	rel_int	65	200	y	n	19:40	10	65	3	289.92	291.92	0.77	0.15
38	Unk	CL4-PCB-43/49	rel_int	65	200	y	n	19:53	10	65	3	289.92	291.92	0.77	0.15
39	Unk	CL4-PCB-48/75	rel_int	65	200	y	n	20:09	10	65	3	289.92	291.92	0.77	0.15
40	Unk	CL4-PCB-47	rel_int	65	100	y	n	20:03	6	65	3	289.92	291.92	0.77	0.15
41	Unk	CL4-PCB-65/62	rel_int	65	200	y	n	20:20	15	65	3	289.92	291.92	0.77	0.15
42	Unk	CL4-PCB-44	rel_int	65	100	y	n	20:44	6	65	3	289.92	291.92	0.77	0.15
43	Unk	CL4-PCB-42/59	rel_int	65	200	y	n	20:55	10	65	3	289.92	291.92	0.77	0.15
44	Unk	CL4-PCB-64/71/41/72	rel_int	65	400	y	n	21:27	15	65	4	289.92	291.92	0.77	0.15
45	Unk	CL4-PCB-40	rel_int	65	100	y	n	21:50	6	65	4	289.92	291.92	0.77	0.15
46	Unk	CL4-PCB-68	rel_int	65	100	y	n	21:43	6	65	4	289.92	291.92	0.77	0.15

Table 7b. (continued)

Ent	Type	Name	Method	Std	Amo ng	1	2	RT	Win. sec	Std.	Fn	m1	m2	m1/m2	Tol.
47	Unk	CL4-PCB-57	rel_int	65	100	y	n	22:13	6	65	4	289.92	291.92	0.77	0.15
48	Unk	CL4-PCB-58	rel_int	65	100	y	n	22:35	6	65	4	289.92	291.92	0.77	0.15
49	Unk	CL4-PCB-67	rel_int	65	100	y	n	22:29	6	65	4	289.92	291.92	0.77	0.15
50	Unk	CL4-PCB-63	rel_int	65	100	y	n	22:45	6	65	4	289.92	291.92	0.77	0.15
51	Unk	CL4-PCB-74/61	rel_int	65	200	y	n	23:01	15	65	4	289.92	291.92	0.77	0.15
52	Unk	CL4-PCB-70	rel_int	65	100	y	n	23:12	6	65	4	289.92	291.92	0.77	0.15
53	Unk	CL4-PCB-76/66	rel_int	65	200	y	n	23:20	15	65	4	289.92	291.92	0.77	0.15
54	Unk	CL4-PCB-55	rel_int	65	100	y	n	23:50	6	65	4	289.92	291.92	0.77	0.15
55	Unk	CL4-PCB-56	rel_int	65	100	y	n	24:17	6	65	4	289.92	291.92	0.77	0.15
56	Unk	CL4-PCB-60	rel_int	65	100	y	n	24:18	6	65	4	289.92	291.92	0.77	0.15
57	Unk	CL4-PCB-80	rel_int	65	100	y	n	23:38	6	65	4	289.92	291.92	0.77	0.15
58	Unk	CL4-PCB-79	rel_int	65	100	y	n	25:22	6	65	4	289.92	291.92	0.77	0.15
59	Unk	CL4-PCB-78	rel_int	65	100	y	n	25:59	6	65	4	289.92	291.92	0.77	0.15
60	Unk	CL4-PCB-81	rel_int	65	100	y	n	26:29	6	65	4	289.92	291.92	0.77	0.15
61	Unk	CL4-PCB-77	rel_int	65	100	y	n	27:03	6	65	4	289.92	291.92	0.77	0.15
62	IS	13C-CL1-PCB-3	rel_int	66	100	n	y	10:56	10	66	1	200.08	202.08	3.13	0.15
63	IS	13C-CL2-PCB-15	rel_int	66	100	n	y	15:17	10	66	2	234.04	236.04	1.56	0.15
64	IS	13C-CL3-PCB-28	rel_int	66	100	n	y	17:38	10	66	3	268	270	1.04	0.15
65	IS	13C-CL4-PCB-77	rel_int	66	100	n	y	27:02	10	66	4	301.96	303.96	0.77	0.15
66	RS/RT	13C-CL4-PCB-52	abs_int		500	n	y	19:39	25		3	301.96	303.96	0.77	0.15
67	C/Up	13C-CL4-PCB-81	rel_int	66	50	y	y	26:28	10	66	4	301.96	303.96	0.77	0.15

Part 2. Analyte table 1668XAB-DB1-C for Cl5s

1	Unk	CL5-PCB-104	rel_int	30	100	y	n	20:36	6	30	3	325.88	327.88	1.55	0.15
2	Unk	CL5-PCB-96	rel_int	30	100	y	n	21:40	6	30	4	325.88	327.88	1.55	0.15
3	Unk	CL5-PCB-103	rel_int	30	100	y	n	22:14	6	30	4	325.88	327.88	1.55	0.15
4	Unk	CL5-PCB-94	rel_int	30	100	y	n	22:58	6	30	4	325.88	327.88	1.55	0.15
5	Unk	CL5-PCB-98/102/93/95	rel_int	30	400	y	n	23:27	15	30	4	325.88	327.88	1.55	0.15
6	Unk	CL5-PCB-100	rel_int	30	100	y	n	22:33	6	30	4	325.88	327.88	1.55	0.15
7	Unk	CL5-PCB-88	rel_int	30	100	y	n	23:43	6	30	4	325.88	327.88	1.55	0.15
8	Unk	CL5-PCB-91	rel_int	30	100	y	n	23:49	6	30	4	325.88	327.88	1.55	0.15
9	Unk	CL5-PCB-84/92/89	rel_int	30	300	y	n	24:44	15	30	4	325.88	327.88	1.55	0.15
10	Unk	CL5-PCB-121	rel_int	30	100	y	n	23:58	6	30	4	325.88	327.88	1.55	0.15
11	Unk	CL5-PCB-90/101	rel_int	30	200	y	n	25:05	10	30	4	325.88	327.88	1.55	0.15
12	Unk	CL5-PCB-113/99	rel_int	30	200	y	n	25:21	15	30	4	325.88	327.88	1.55	0.15
13	Unk	CL5-PCB-83/112	rel_int	30	200	y	n	25:58	10	30	4	325.88	327.88	1.55	0.15
14	Unk	CL5-PCB-108	rel_int	30	100	y	n	26:06	6	30	4	325.88	327.88	1.55	0.15
15	Unk	CL5-PCB-119	rel_int	30	100	y	n	25:50	6	30	4	325.88	327.88	1.55	0.15
16	Unk	CL5-PCB-86	rel_int	30	100	y	n	26:25	6	30	4	325.88	327.88	1.55	0.15
17	Unk	CL5-PCB-97	rel_int	30	100	y	n	26:18	6	30	4	325.88	327.88	1.55	0.15
18	Unk	CL5-PCB-117/125/87	rel_int	30	300	y	n	26:34	10	30	4	325.88	327.88	1.55	0.15
19	Unk	CL5-PCB-115/116/111/85	rel_int	30	400	y	n	26:48	15	30	4	325.88	327.88	1.55	0.15
20	Unk	CL5-PCB-82	rel_int	30	100	y	n	27:46	6	30	4	325.88	327.88	1.55	0.15
21	Unk	CL5-PCB-120/110	rel_int	30	200	y	n	27:13	10	30	4	325.88	327.88	1.55	0.15
22	Unk	CL5-PCB-124/107/109	rel_int	30	300	y	n	28:38	15	30	5	325.88	327.88	1.55	0.15

Table 7b. (continued)

Ent	Type	Name	Method	Std	Amo	1	2	RT	Win.	Std.	Fn	m1	m2	m1/m2	Tol.
23	Unk	CL5-PCB-123	rel_int	30	100	y	n	28:51	6	30	5	325.88	327.88	1.55	0.15
24	Unk	CL5-PCB-118/106	rel_int	30	200	y	n	29:03	10	30	5	325.88	327.88	1.55	0.15
25	Unk	CL5-PCB-122	rel_int	30	100	y	n	29:47	6	30	5	325.88	327.88	1.55	0.15
26	Unk	CL5-PCB-114	rel_int	30	100	y	n	29:39	6	30	5	325.88	327.88	1.55	0.15
27	Unk	CL5-PCB-105	rel_int	31	100	y	n	30:30	6	31	5	325.88	327.88	1.55	0.15
28	Unk	CL5-PCB-127	rel_int	32	100	y	n	30:56	6	32	5	325.88	327.88	1.55	0.15
29	Unk	CL5-PCB-126	rel_int	32	100	y	n	32:48	6	32	5	325.88	327.88	1.55	0.15
30	IS	13C-CL5-PCB-118	rel_int	33	100	n	y	29:01	10	33	5	335.92	337.92	0.63	0.15
31	IS	13C-CL5-PCB-105	rel_int	33	100	n	y	30:29	10	33	5	335.92	337.92	0.63	0.15
32	IS	13C-CL5-PCB-126	rel_int	33	100	n	y	32:47	10	33	5	335.92	337.92	0.63	0.15
33	RS/RT	13C-CL5-PCB-101	abs_int		500	n	y	25:05	25		4	335.92	337.92	0.63	0.15
34	C/Up	13C-CL5-PCB-111	rel_int	33	250	y	y	26:46	10	33	4	335.92	337.92	0.63	0.15

Part 3. Analyte table 1668XAC-DB1-C for Cl6s

Ent	Type	Name	Method	Std	Amo	1	2	RT	Win.	Std.	Fn	m1	m2	m1/m2	Tol.
1	Unk	CL6-PCB-155	rel_int	34	100	y	n	24:38	6	34	4	359.84	361.84	1.24	0.15
2	Unk	CL6-PCB-152	rel_int	34	100	y	n	26:14	6	34	4	359.84	361.84	1.24	0.15
3	Unk	CL6-PCB-150	rel_int	34	100	y	n	25:49	6	34	4	359.84	361.84	1.24	0.15
4	Unk	CL6-PCB-136	rel_int	34	100	y	n	26:59	6	34	4	359.84	361.84	1.24	0.15
5	Unk	CL6-PCB-145	rel_int	34	100	y	n	26:40	6	34	4	359.84	361.84	1.24	0.15
6	Unk	CL6-PCB-148	rel_int	34	100	y	n	27:11	6	34	4	359.84	361.84	1.24	0.15
7	Unk	CL6-PCB-151	rel_int	34	100	y	n	28:17	6	34	5	359.84	361.84	1.24	0.15
8	Unk	CL6-PCB-135/144	rel_int	34	200	y	n	28:34	10	34	5	359.84	361.84	1.24	0.15
9	Unk	CL6-PCB-154	rel_int	34	100	y	n	27:41	6	34	4	359.84	361.84	1.24	0.15
10	Unk	CL6-PCB-147	rel_int	34	100	y	n	28:43	6	34	5	359.84	361.84	1.24	0.15
11	Unk	CL6-PCB-139/149	rel_int	34	200	y	n	29:00	6	34	5	359.84	361.84	1.24	0.15
12	Unk	CL6-PCB-134/143	rel_int	34	200	y	n	29:35	10	34	5	359.84	361.84	1.24	0.15
13	Unk	CL6-PCB-140	rel_int	34	100	y	n	29:10	6	34	5	359.84	361.84	1.24	0.15
14	Unk	CL6-PCB-131	rel_int	34	100	y	n	29:51	6	34	5	359.84	361.84	1.24	0.15
15	Unk	CL6-PCB-133/142	rel_int	34	200	y	n	29:58	8	34	5	359.84	361.84	1.24	0.15
16	Unk	CL6-PCB-165/146	rel_int	34	200	y	n	30:22	8	34	5	359.84	361.84	1.24	0.15
17	Unk	CL6-PCB-132/161	rel_int	34	200	y	n	30:33	8	34	5	359.84	361.84	1.24	0.15
18	Unk	CL6-PCB-153	rel_int	34	100	y	n	30:47	6	34	5	359.84	361.84	1.24	0.15
19	Unk	CL6-PCB-168	rel_int	34	100	y	n	31:00	6	34	5	359.84	361.84	1.24	0.15
20	Unk	CL6-PCB-141	rel_int	34	100	y	n	31:31	6	34	5	359.84	361.84	1.24	0.15
21	Unk	CL6-PCB-130	rel_int	34	100	y	n	31:58	6	34	5	359.84	361.84	1.24	0.15
22	Unk	CL6-PCB-137	rel_int	34	100	y	n	31:53	6	34	5	359.84	361.84	1.24	0.15
23	Unk	CL6-PCB-138/163/164	rel_int	34	300	y	n	32:23	8	34	5	359.84	361.84	1.24	0.15
24	Unk	CL6-PCB-129	rel_int	34	100	y	n	32:50	6	34	5	359.84	361.84	1.24	0.15
25	Unk	CL6-PCB-158/160	rel_int	34	200	y	n	32:35	8	34	5	359.84	361.84	1.24	0.15
26	Unk	CL6-PCB-166	rel_int	34	100	y	n	33:16	6	34	5	359.84	361.84	1.24	0.15
27	Unk	CL6-PCB-128	rel_int	34	100	y	n	33:53	6	34	5	359.84	361.84	1.24	0.15

Table 7b. (continued)

Ent	Type	Name	Method	Std	Amo ng	1	2	RT	Win. sec	Std.	Fn	m1	m2	m1/m2	Tol.
28	Unk	CL6-PCB-159	rel_int	34	100	y	n	33:44	6	34	5	359.84	361.84	1.24	0.15
29	Unk	CL6-PCB-162	rel_int	34	100	y	n	34:03	6	34	5	359.84	361.84	1.24	0.15
30	Unk	CL6-PCB-167	rel_int	34	100	y	n	34:26	6	34	5	359.84	361.84	1.24	0.15
31	Unk	CL6-PCB-156	rel_int	35	100	y	n	35:44	10	35	5	359.84	361.84	1.24	0.15
32	Unk	CL6-PCB-157	rel_int	36	100	y	n	36:00	10	36	5	359.84	361.84	1.24	0.15
33	Unk	CL6-PCB-169	rel_int	37	100	y	n	38:22	6	37	5	359.84	361.84	1.24	0.15
34	IS	13C-CL6-PCB-167	rel_int	38	100	n	y	34:25	10	38	5	371.88	373.89	1.24	0.15
35	IS	13C-CL6-PCB-156	rel_int	38	100	n	y	35:43	10	38	5	371.88	373.88	1.24	0.15
36	IS	13C-CL6-PCB-157	rel_int	38	100	n	y	35:59	10	38	5	371.88	373.88	1.24	0.15
37	IS	13C-CL6-PCB-169	rel_int	38	100	n	y	38:21	10	38	5	371.88	373.89	1.24	0.15
38	RS/RT	13C-CL6-PCB-138	abs_int		500	n	y	32:20	25		5	371.88	373.88	1.24	0.15

Part4. Analyte table 1668XD-DB1-C for Cl7 to Cl10

1	Unk	CL7-PCB-188	rel_int	38	100	y	n	30:22	6	38	5	393.80	395.80	1.05	0.15
2	Unk	CL7-PCB-179	rel_int	38	100	y	n	31:35	6	38	5	393.80	395.80	1.05	0.15
3	Unk	CL7-PCB-184	rel_int	38	100	y	n	30:48	6	38	5	393.80	395.80	1.05	0.15
4	Unk	CL7-PCB-176	rel_int	38	100	y	n	32:03	6	38	5	393.80	395.80	1.05	0.15
5	Unk	CL7-PCB-186	rel_int	38	100	y	n	32:37	6	38	5	393.80	395.80	1.05	0.15
6	Unk	CL7-PCB-178	rel_int	38	100	y	n	33:15	6	38	5	393.80	395.80	1.05	0.15
7	Unk	CL7-PCB-175	rel_int	38	100	y	n	33:37	6	38	5	393.80	395.80	1.05	0.15
8	Unk	CL7-PCB-187/182	rel_int	38	200	y	n	33:48	8	38	5	393.80	395.80	1.05	0.15
9	Unk	CL7-PCB-183	rel_int	38	100	y	n	34:08	6	38	5	393.80	395.80	1.05	0.15
10	Unk	CL7-PCB-185	rel_int	38	100	y	n	34:47	6	38	5	393.80	395.80	1.05	0.15
11	Unk	CL7-PCB-174/181	rel_int	38	200	y	n	35:11	10	38	5	393.80	395.80	1.05	0.15
12	Unk	CL7-PCB-177	rel_int	38	100	y	n	35:26	6	38	5	393.80	395.80	1.05	0.15
13	Unk	CL7-PCB-171	rel_int	38	100	y	n	35:44	6	38	5	393.80	395.80	1.05	0.15
14	Unk	CL7-PCB-173	rel_int	38	100	y	n	36:08	6	38	5	393.80	395.80	1.05	0.15
15	Unk	CL7-PCB-172	rel_int	38	100	y	n	36:46	6	38	5	393.80	395.80	1.05	0.15
16	Unk	CL7-PCB-192	rel_int	38	100	y	n	36:56	6	38	5	393.80	395.80	1.05	0.15
17	Unk	CL7-PCB-193	rel_int	38	100	y	n	37:24	6	38	5	393.80	395.80	1.05	0.15
18	Unk	CL7-PCB-180	rel_int	38	100	y	n	37:11	6	38	5	393.80	395.80	1.05	0.15
19	Unk	CL7-PCB-191	rel_int	38	100	y	n	37:38	6	38	5	393.80	395.80	1.05	0.15
20	Unk	CL7-PCB-170	rel_int	38	100	y	n	38:49	6	38	5	393.80	395.80	1.05	0.15
21	Unk	CL7-PCB-190	rel_int	38	100	y	n	39:03	6	38	5	393.80	395.80	1.05	0.15
22	Unk	CL7-PCB-189	rel_int	39	100	y	n	40:57	6	39	5	393.80	395.80	1.05	0.15
23	Unk	CL8-PCB-202	rel_int	40	150	y	n	36:00	6	40	5	427.76	429.76	0.89	0.15
24	Unk	CL8-PCB-201	rel_int	40	150	y	n	36:30	6	40	5	427.76	429.76	0.89	0.15
25	Unk	CL8-PCB-204	rel_int	40	150	y	n	36:40	6	40	5	427.76	429.76	0.89	0.15
26	Unk	CL8-PCB-197	rel_int	40	150	y	n	36:59	6	40	5	427.76	429.76	0.89	0.15
27	Unk	CL8-PCB-200	rel_int	40	150	y	n	37:54	7	40	5	427.76	429.76	0.89	0.15
28	Unk	CL8-PCB-198	rel_int	40	150	y	n	39:39	6	40	5	427.76	429.76	0.89	0.15
29	Unk	CL8-PCB-199	rel_int	40	150	y	n	39:49	6	40	5	427.76	429.76	0.89	0.15
30	Unk	CL8-PCB-196/203	rel_int	40	300	y	n	40:11	8	40	5	427.76	429.76	0.89	0.15

Table 7b. (continued)

Ent	Type	Name	Method	Std	Amo ng	1	2	RT	Win. sec	Std.	Fn	m1	m2	m1/m2	Tol.
31	Unk	CL8-PCB-195	rel_int	40	150	y	n	41:52	6	40	6	427.76	429.76	0.89	0.15
32	Unk	CL8-PCB-194	rel_int	40	150	y	n	43:24	6	40	6	427.76	429.76	0.89	0.15
33	Unk	CL8-PCB-205	rel_int	40	150	y	n	43:50	6	40	6	427.76	429.76	0.89	0.15
34	Unk	CL9-PCB-208	rel_int	41	150	y	n	42:08	6	41	6	461.72	463.72	0.78	0.15
35	Unk	CL9-PCB-207	rel_int	41	150	y	n	42:39	6	41	6	461.72	463.72	0.78	0.15
36	Unk	CL9-PCB-206	rel_int	41	150	y	n	46:01	7	41	6	461.72	463.72	0.78	0.15
37	Unk	CL10-PCB-209	rel_int	42	150	y	n	48:05	6	42	6	495.69	497.68	0.69	0.15
38	IS	13C-CL7-PCB-180	rel_int	43	100	n	y	37:10	10	43	5	405.80	407.84	1.05	0.15
39	IS	13C-CL7-PCB-189	rel_int	43	100	n	y	40:58	10	43	5	405.80	407.84	1.05	0.15

Table 8. Theoretical Ion Abundance Ratios and QC limits for PCB congeners

Chlorine Atoms	m/z forming ratio	Theoretical Ratio	QC limits	
			Lower	Upper
1.00	m/m+2	3.13	2.66	3.60
2.00	m/(m+2)	1.56	1.33	1.79
3.00	m/(m+2)	1.04	0.88	1.20
4.00	m/(m+2)	0.77	0.65	0.89
5.00	(m+2)/(m+4)	1.55	1.32	1.78
6.00	(m+2)/(m+4)	1.24	1.05	1.43
7.00	(m+2)/(m+4)	1.05	0.89	1.21
8.00	(m+2)/(m+4)	0.89	0.76	1.02
9.00	(m+2)/(m+4)	0.77	0.65	0.89
10.00	(m+2)/(m+4)	0.69	0.59	0.79

**Table 9a. Retention Times (RT) and peak separations for each of the five Series 2
1668 Full Congener standards on a 30m Octyl column**

Series 2 Standard ID	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m (min:sec)	Separation from Preceding isomer (sec)
A2	2	1	16:11	
A2	10	2	16:55	
A2	9	2	18:59	124
A2	6	2	19:29	30
A2	8	2	19:59	30
A2	14	2	21:45	106
A2	11	2	22:46	61
A2	30	3	22:19	
A2	27	3	23:10	51
A2	32	3	24:05	55
A2	34	3	25:21	76
A2	26	3	25:51	30
A2	31	3	26:32	41
A2	33	3	27:06	34
A2	36	3	29:09	123
A2	38	3	30:12	63
A2	35	3	30:46	34
A2	50	4	26:11	
A2	45	4	27:01	50
A2	52	4	28:48	107
A2	49	4	29:19	31
A2	75	4	30:12	53
A2	41	4	30:56	44
A2	72	4	32:02	66
A2	57	4	32:49	47
A2	63	4	33:38	49
A2	66	4	34:20	42
A2	79	4	37:19	179
A2	78	4	37:58	39
A2	81	4	38:28	30
A2	96	5	30:22	
A2	103	5	32:15	113
A2	95	5	33:09	54
A2	88	5	33:56	47
A2	89	5	34:48	52
A2	92	5	35:33	45
A2	113	5	36:05	32
A2	83	5	36:43	38
A2	119	5	37:16	33
A2	87	5	37:30	14
A2	85	5	38:00	30
A2	82	5	38:48	48
A2	120	5	39:29	41
A2	124	5	40:43	74
A2	106	5	41:17	34
A2	122	5	41:56	39
A2	105	5	42:51	55

Table 9a. (continued)

Series 2 Standard	Congener ID	IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
				(min:sec)	(sec)
A2	127		5	44:13	82
A2	152		6	36:12	
A2	136		6	36:49	37
A2	148		6	38:32	103
A2	151		6	39:13	41
A2	144		6	39:51	38
A2	143		6	40:35	44
A2	142		6	41:19	44
A2	133		6	42:03	44
A2	161		6	42:50	47
A2	153		6	43:21	31
A2	130		6	44:05	44
A2	129		6	44:52	47
A2	166		6	46:04	72
A2	159		6	47:03	59
A2	167		6	47:52	49
A2	156		6	49:10	78
A2	179		7	42:25	
A2	176		7	43:22	57
A2	178		7	45:09	107
A2	175		7	45:53	44
A2	183		7	46:46	53
A2	177		7	47:38	52
A2	171		7	48:17	39
A2	172		7	49:51	94
A2	191		7	50:57	66
A2	170		7	51:58	61
A2	190		7	52:32	34
A2	201/200		8	48:33	
A2	204		8	49:13	40
A2	200/199		8	49:43	30
A2	198		8	52:34	171
A2	196		8	53:17	43
A2	195		8	54:58	101
A2	194		8	57:22	144
A2	207		9	55:38	
B2	7		2	19:10	
B2	5		2	19:54	44
B2	12		2	23:09	195
B2	18		3	22:27	
B2	24		3	23:17	50
B2	23		3	25:28	131
B2	28		3	26:52	84
B2	22		3	27:35	43
B2	39		3	29:34	119
B2	53		4	26:14	
B2	51		4	27:02	48
B2	73		4	28:55	113
B2	48		4	29:37	42
B2	62		4	30:14	37
B2	71		4	31:02	48
B2	68		4	32:21	79

Table 9a. (continued)

Series 2 Standard	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
B2	58	4	33:08	(min:sec) (sec) 47
B2	61	4	33:51	43
B2	55	4	34:32	41
B2	60	4	35:25	53
B2	94	5	32:37	
B2	100	5	33:11	34
B2	91	5	33:59	48
B2	121	5	35:00	61
B2	90	5	36:07	67
B2	99	5	36:45	38
B2	108/109	5	37:16	31
B2	117	5	38:00	44
B2	111	5	38:56	56
B2	107/108	5	40:43	107
B2	118	5	41:27	44
B2	114	5	42:03	36
B2	150	6	36:23	
B2	145	6	37:05	42
B2	135	6	39:20	135
B2	149	6	40:14	54
B2	139	6	40:49	35
B2	132	6	41:41	52
B2	165	6	42:25	44
B2	168	6	43:24	59
B2	137	6	44:17	53
B2	160	6	44:56	39
B2	128	6	46:13	77
B2	162	6	47:22	69
B2	157	6	49:13	111
B2	184	7	42:48	
B2	186	7	43:51	63
B2	187	7	46:05	134
B2	185	7	46:56	51
B2	181	7	47:55	59
B2	192	7	50:08	133
B2	197	8	49:29	
B2	199/201	8	52:35	186
B2	203	8	53:29	54
C2	13	2	23:10	
C2	17	3	22:53	
C2	29	3	25:51	178
C2	20	3	26:54	63
C2	46	4	27:22	
C2	65	4	29:52	150
C2	59	4	30:17	25
C2	40	4	31:02	45
C2	67	4	33:16	134
C2	76	4	33:58	42
C2	80	4	35:36	98
C2	93	5	33:18	
C2	84	5	34:22	64
C2	101	5	36:12	110

Table 9a. (continued)

Series 2 Standard ID	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
			(min:sec)	(sec)
C2	112	5	36:54	42
C2	86	5	37:25	31
C2	116	5	38:06	41
C2	109/107	5	40:58	172
C2	154	6	39:24	
C2	147	6	40:16	52
C2	140	6	40:51	35
C2	146	6	42:42	111
C2	141	6	43:41	59
C2	164	6	44:30	49
C2	158	6	45:09	39
C2	182	7	46:21	
C2	174	7	47:05	44
C2	173	7	48:14	69
C2	193	7	50:32	138
D2	25	3	26:08	
D2	21	3	27:01	53
D2	69	4	29:14	
D2	47	4	29:56	42
D2	42	4	30:31	35
D2	64	4	31:17	46
D2	70	4	33:58	161
D2	102	5	33:26	
D2	97	5	37:25	239
D2	115	5	38:22	57
D2	123	5	41:06	164
D2	134	6	40:32	
D2	131	6	41:08	36
D2	163	6	44:47	219
D2	180	7	50:33	
E2	1	1	13:46	
E2	3	1	16:23	157
E2	4	2	16:47	
E2	15	2	23:33	406
E2	19	3	20:23	
E2	16	3	23:28	185
E2	37	3	31:18	470
E2	54	4	23:55	
E2	43	4	29:06	311
E2	44	4	30:00	54
E2	74	4	34:00	240
E2	56	4	35:07	67
E2	77	4	39:07	240
E2	104	5	29:53	
E2	98	5	33:29	216
E2	125	5	37:25	236
E2	110	5	38:23	58
E2	126	5	46:02	459
E2	155	6	35:48	
E2	138	6	44:47	539
E2	169	6	52:38	471
E2	188	7	41:58	

Table 9a. (continued)

Series 2 Standard ID	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
E2	189	7	55:11	(sec) 793
E2	202	8	47:35	
E2	205	8	57:52	617
E2	208	9	54:35	
E2	206	9	59:43	308
E2	209	10	61:22	

Table 9b. Congener retention times (RTs) and peak separations on a 30m Octyl column sorted by level of chlorination then retention time

Series 2 Standard ID	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m (min:sec)	Separation from Preceding isomer (sec)
E2	1	1	13:46	
A2	2	1	16:11	145
E2	3	1	16:23	12
E2	4	2	16:47	
A2	10	2	16:55	8
A2	9	2	18:59	124
B2	7	2	19:10	11
A2	6	2	19:29	19
B2	5	2	19:54	25
A2	8	2	19:59	5
A2	14	2	21:45	106
A2	11	2	22:46	61
B2	12	2	23:09	23
C2	13	2	23:10	1
E2	15	2	23:33	23
A2	32	3	24:05	
A2	34	3	25:21	116
A2	26	3	25:51	8
A2	31	3	26:32	26
A2	33	3	27:06	17
A2	36	3	29:09	7
A2	38	3	30:12	11
A2	35	3	30:46	37
B2	23	3	25:28	76
B2	28	3	26:52	7
B2	22	3	27:35	23
B2	39	3	29:34	0
C2	29	3	25:51	17
C2	20	3	26:54	24
D2	25	3	26:08	20
D2	21	3	27:01	2
E2	37	3	31:18	7
E2	19	3	20:23	5
A2	30	3	22:19	29
B2	18	3	22:27	94
C2	17	3	22:53	25
A2	27	3	23:10	38
B2	24	3	23:17	34
E2	16	3	23:28	32
A2	50	4	26:11	
A2	45	4	27:01	136
A2	52	4	28:48	3
A2	49	4	29:19	47
A2	75	4	30:12	1
A2	41	4	30:56	20
A2	72	4	32:02	86
A2	57	4	32:49	7

Table 9b. (continued)

Series 2 Standard	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
A2	63	4	33:38	11
A2	66	4	34:20	8
A2	79	4	37:19	5
A2	78	4	37:58	18
A2	81	4	38:28	15
B2	53	4	26:14	4
B2	51	4	27:02	4
B2	73	4	28:55	12
B2	48	4	29:37	2
B2	62	4	30:14	3
B2	71	4	31:02	14
B2	68	4	32:21	25
B2	58	4	33:08	6
B2	61	4	33:51	0
B2	55	4	34:32	15
B2	60	4	35:25	45
C2	46	4	27:22	19
C2	65	4	29:52	28
C2	59	4	30:17	19
C2	40	4	31:02	8
C2	67	4	33:16	22
C2	76	4	33:58	13
C2	80	4	35:36	7
D2	69	4	29:14	0
D2	47	4	29:56	2
D2	42	4	30:31	20
D2	64	4	31:17	12
D2	70	4	33:58	35
E2	43	4	29:06	18
E2	44	4	30:00	11
E2	74	4	34:00	103
E2	56	4	35:07	39
E2	77	4	39:07	30
E2	54	4	23:55	39
A2	96	5	30:22	
A2	103	5	32:15	29
A2	95	5	33:09	113
A2	88	5	33:56	22
A2	89	5	34:48	32
A2	92	5	35:33	2
A2	113	5	36:05	7
A2	83	5	36:43	8
A2	119	5	37:16	3
A2	87	5	37:30	27
A2	85	5	38:00	3
A2	82	5	38:48	23
A2	120	5	39:29	26
A2	124	5	40:43	12
A2	106	5	41:17	33
A2	122	5	41:56	32
A2	105	5	42:51	2
A2	127	5	44:13	5

Table 9b. (continued)

Series 2 Standard	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
B2	94	5	32:37	31
B2	100	5	33:11	2
B2	91	5	33:59	9
B2	121	5	35:00	22
B2	90	5	36:07	0
B2	99	5	36:45	9
B2	108/109	5	37:16	0
B2	117	5	38:00	0
B2	111	5	38:56	5
B2	107/108	5	40:43	30
B2	118	5	41:27	0
B2	114	5	42:03	6
C2	93	5	33:18	16
C2	84	5	34:22	1
C2	101	5	36:12	25
C2	112	5	36:54	8
C2	86	5	37:25	33
C2	116	5	38:06	74
C2	109/107	5	40:58	0
D2	102	5	33:26	15
D2	97	5	37:25	8
D2	115	5	38:22	11
D2	123	5	41:06	10
E2	104	5	29:53	29
E2	98	5	33:29	7
E2	125	5	37:25	48
E2	110	5	38:23	82
E2	126	5	46:02	109
A2	152	6	36:12	
A2	136	6	36:49	24
A2	148	6	38:32	11
A2	151	6	39:13	26
A2	144	6	39:51	16
A2	143	6	40:35	87
A2	142	6	41:19	41
A2	133	6	42:03	7
A2	161	6	42:50	4
A2	153	6	43:21	27
A2	130	6	44:05	23
A2	129	6	44:52	2
A2	166	6	46:04	16
A2	159	6	47:03	3
A2	167	6	47:52	14
A2	156	6	49:10	2
B2	150	6	36:23	17
B2	145	6	37:05	11
B2	135	6	39:20	22
B2	149	6	40:14	22
B2	139	6	40:49	22
B2	132	6	41:41	17
B2	165	6	42:25	8
B2	168	6	43:24	31

Table 9b. (continued)

Series 2 Standard	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
B2	137	6	44:17	(min:sec) (sec) 3
B2	160	6	44:56	17
B2	128	6	46:13	24
B2	162	6	47:22	12
B2	157	6	49:13	13
C2	154	6	39:24	17
C2	147	6	40:16	0
C2	140	6	40:51	5
C2	146	6	42:42	4
C2	141	6	43:41	13
C2	164	6	44:30	55
C2	158	6	45:09	9
D2	134	6	40:32	50
D2	131	6	41:08	19
D2	163	6	44:47	30
E2	155	6	35:48	78
E2	138	6	44:47	3
E2	169	6	52:38	205
A2	179	7	42:25	
A2	176	7	43:22	27
A2	178	7	45:09	23
A2	175	7	45:53	34
A2	183	7	46:46	29
A2	177	7	47:38	78
A2	171	7	48:17	44
A2	172	7	49:51	12
A2	191	7	50:57	16
A2	170	7	51:58	25
A2	190	7	52:32	10
B2	184	7	42:48	9
B2	186	7	43:51	33
B2	187	7	46:05	17
B2	185	7	46:56	19
B2	181	7	47:55	3
B2	192	7	50:08	94
C2	182	7	46:21	17
C2	174	7	47:05	24
C2	173	7	48:14	1
C2	193	7	50:32	24
D2	180	7	50:33	61
E2	188	7	41:58	34
E2	189	7	55:11	159
A2	201/200	8	48:33	
A2	204	8	49:13	58
A2	200/199	8	49:43	40
A2	198	8	52:34	16
A2	196	8	53:17	14
A2	195	8	54:58	171
A2	194	8	57:22	1
B2	197	8	49:29	42
B2	199/201	8	52:35	12
B2	203	8	53:29	89

Table 9b. (continued)

Series 2 Standard ID	Congener IUPAC # or IUPAC/BZ#	# Chlorines	RT Octyl 30m	Separation from Preceding isomer
E2	202	8	47:35	(sec) 144
E2	205	8	57:52	30
A2	207	9	55:38	
E2	208	9	54:35	63
E2	206	9	59:43	245
E2	209	10	61:22	

**Table 10a. Retention Times (RT) and peak separations for each of the five Series 2
1668 Full Congener standards on a 30m DB-1 column**

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
A2	2	1	10:22	
A2	10	2	11:10	
A2	9	2	12:08	58.0
A2	6	2	12:31	23.0
A2	8	2	12:43	12.0
A2	14	2	13:36	53.0
A2	11	2	14:11	35.0
A2	30	3	14:06	
A2	27	3	15:06	60.0
A2	32	3	15:29	23.0
A2	34	3	16:03	34.0
A2	26	3	16:29	26.0
A2	31	3	16:52	23.0
A2	33	3	17:24	32.0
A2	36	3	18:16	52.0
A2	38	3	19:12	56.0
A2	35	3	19:41	29.0
A2	50	4	16:55	
A2	45	4	18:00	65.0
A2	52	4	18:51	51.0
A2	49	4	19:00	9.0
A2	75	4	19:20	20.0
A2	72	4	20:36	76.0
A2	41	4	20:39	3.0
A2	57	4	21:21	42.0
A2	63	4	21:51	30.0
A2	66	4	22:29	38.0
A2	79	4	24:27	118.0
A2	78	4	25:04	37.0
A2	81	4	25:32	28.0
A2	96	5	20:48	
A2	103	5	21:22	34.0
A2	95	5	22:34	72.0
A2	88	5	22:49	15.0
A2	92	5	23:50	61.0
A2	89	5	23:53	3.0
A2	113	5	24:23	30.0
A2	119	5	24:54	31.0

Table 10a. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
A2	83	5	25:02	8.0
A2	87	5	25:38	36.0
A2	85	5	25:51	13.0
A2	120	5	26:12	21.0
A2	82	5	26:48	36.0
A2	124	5	27:36	48.0
A2	106	5	28:04	28.0
A2	122	5	28:48	44.0
A2	105	5	29:30	42.0
A2	127	5	29:57	27.0
A2	152	6	25:17	
A2	136	6	26:01	44.0
A2	148	6	26:14	13.0
A2	151	6	27:18	64.0
A2	144	6	27:38	20.0
A2	143	6	28:34	56.0
A2	142	6	28:59	25.0
A2	133	6	28:59	0.0
A2	161	6	29:32	33.0
A2	153	6	29:48	16.0
A2	130	6	30:57	69.0
A2	129	6	31:48	51.0
A2	166	6	32:13	25.0
A2	159	6	32:43	30.0
A2	167	6	33:23	40.0
A2	156	6	34:40	77.0
A2	179	7	30:33	
A2	176	7	31:01	28.0
A2	178	7	32:14	73.0
A2	175	7	32:33	19.0
A2	183	7	33:6	33.0
A2	177	7	34:22	76.0
A2	171	7	34:40	18.0
A2	172	7	35:41	61.0
A2	191	7	36:34	53.0
A2	170	7	37:44	70.0
A2	190	7	37:56	12.0
A2	201	8	35:25	
A2	204	8	35:36	11.0
A2	200	8	36:49	73.0
A2	198	8	38:34	105.0

Table 10a. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
A2	196	8	39:05	31.0
A2	195	8	40:45	100.0
A2	194	8	42:16	91.0
A2	207	9	41:32	
B2	7	2	12:09	
B2	5	2	12:46	37.0
B2	12	2	14:27	101.0
B2	18	3	14:36	
B2	24	3	15:06	30.0
B2	23	3	16:07	61.0
B2	28	3	16:55	48.0
B2	22	3	17:43	48.0
B2	39	3	18:37	54.0
B2	53	4	17:26	
B2	51	4	17:42	16.0
B2	73	4	18:57	75.0
B2	48	4	19:20	23.0
B2	62	4	19:36	16.0
B2	71	4	20:36	60.0
B2	68	4	20:52	16.0
B2	58	4	21:43	51.0
B2	61	4	22:11	28.0
B2	55	4	22:57	46.0
B2	60	4	23:24	27.0
B2	100	5	21:41	
B2	94	5	22:05	24.0
B2	91	5	22:55	50.0
B2	121	5	23:04	9.0
B2	90	5	24:07	63.0
B2	99	5	24:28	21.0
B2	108	5	25:09	41.0
B2	117	5	25:37	28.0
B2	111	5	25:51	14.0
B2	107	5	27:40	109.0
B2	118	5	28:04	24.0
B2	114	5	28:38	34.0
B2	150	6	24:52	
B2	145	6	25:42	50.0
B2	135	6	27:31	109.0
B2	149	6	28:01	30.0
B2	139	6	28:01	0.0

Table 10a. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
B2	165	6	29:21	80.0
B2	132	6	29:32	11.0
B2	168	6	29:59	27.0
B2	137	6	30:51	52.0
B2	160	6	31:33	42.0
B2	128	6	32:52	79.0
B2	162	6	33:00	8.0
B2	157	6	34:57	117.0
B2	184	7	29:49	
B2	186	7	31:36	107.0
B2	187	7	32:46	70.0
B2	185	7	33:43	57.0
B2	181	7	34:11	28.0
B2	192	7	35:51	100.0
B2	197	8	35:55	
B2	199	8	38:43	168.0
B2	203	8	39:05	22.0
C2	13	2	14:26	
C2	17	3	14:43	
C2	29	3	16:18	95.0
C2	20	3	17:22	64.0
C2	46	4	18:24	
C2	65	4	19:31	67.0
C2	59	4	20:05	34.0
C2	40	4	20:58	53.0
C2	67	4	21:38	40.0
C2	76	4	22:25	47.0
C2	80	4	22:45	20.0
C2	93	5	22:36	
C2	84	5	23:44	68.0
C2	101	5	24:11	27.0
C2	112	5	25:00	49.0
C2	86	5	25:27	27.0
C2	116	5	25:48	21.0
C2	109	5	27:45	117.0
C2	154	6	26:44	
C2	147	6	27:44	60.0
C2	140	6	28:12	28.0
C2	146	6	29:24	72.0
C2	141	6	30:31	67.0
C2	164	6	31:22	51.0

Table 10a. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
C2	158	6	31:35	13.0
C2	182	7	32:47	
C2	174	7	34:07	80.0
C2	173	7	35:04	57.0
C2	193	7	36:20	76.0
D2	25	3	16:36	
D2	21	3	17:21	45.0
D2	69	4	18:52	
D2	47	4	19:15	23.0
D2	42	4	20:07	52.0
D2	64	4	20:37	30.0
D2	70	4	22:20	103.0
D2	102	5	22:32	
D2	97	5	25:22	170.0
D2	115	5	25:44	22.0
D2	123	5	27:53	129.0
D2	134	6	28:35	
D2	131	6	28:52	17.0
D2	163	6	31:28	156.0
D2	180	7	36:07	
E2	1	1	9:17	
E2	3	1	10:29	72.0
E2	4	2	11:08	
E2	15	2	14:40	212.0
E2	19	3	13:31	
E2	16	3	15:26	115.0
E2	37	3	20:03	277.0
E2	54	4	16:02	
E2	43	4	19:04	182.0
E2	44	4	19:55	51.0
E2	74	4	22:07	132.0
E2	56	4	23:24	77.0
E2	77	4	26:07	163.0
E2	104	5	19:45	
E2	98	5	22:28	163.0
E2	125	5	25:36	188.0
E2	110	5	26:16	40.0
E2	126	5	31:49	333.0
E2	155	6	23:43	
E2	138	6	31:20	457.0
E2	169	6	37:19	359.0

Table 10a. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
E2	188	7	29:22	
E2	189	7	39:51	629.0
E2	202	8	34:56	
E2	205	8	42:44	468.0
E2	208	9	41:03	
E2	206	9	44:52	229.0
E2	209	10	46:55	

Table 10b. Congener retention times (RTs) and peak separations on a 30m DB-1 column sorted by level of chlorination then retention time

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
E2	1	1	9:17	
A2	2	1	10:22	65
E2	3	1	10:29	7
E2	4	2	11:08	
B2	10	2	11:10	2
A2	9	2	12:08	58
B2	7	2	12:09	1
A2	6	2	12:31	22
A2	8	2	12:43	12
A2	5	2	12:46	3
A2	14	2	13:36	50
B2	11	2	14:11	35
C2	13	2	14:26	15
A2	12	2	14:27	1
E2	15	2	14:40	13
E2	19	3	13:31	
C2	30	3	14:06	35
B2	18	3	14:36	30
E2	17	3	14:43	7
C2	27	3	15:06	23
D2	24	3	15:06	0
B2	16	3	15:26	20
B2	32	3	15:29	3
B2	34	3	16:03	34
D2	23	3	16:07	4
A2	29	3	16:18	11
A2	26	3	16:29	11
B2	25	3	16:36	7
C2	31	3	16:52	16
A2	28	3	16:55	3
A2	21	3	17:21	26
A2	20	3	17:22	1
A2	33	3	17:24	2
A2	22	3	17:43	19
A2	36	3	18:16	33
A2	39	3	18:37	21
E2	38	3	19:12	35
A2	35	3	19:41	29

Table 10b. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
B2	37	3	20:03	22
C2	54	4	16:02	
A2	50	4	16:55	53
D2	53	4	17:26	31
E2	51	4	17:42	16
E2	45	4	18:00	18
A2	46	4	18:24	24
C2	69	4	18:52	28
D2	52	4	18:51	-1
B2	73	4	18:57	6
A2	43	4	19:04	7
A2	49	4	19:00	-4
B2	47	4	19:15	15
A2	75	4	19:20	5
B2	48	4	19:20	0
E2	65	4	19:31	11
B2	62	4	19:36	5
E2	44	4	19:55	19
A2	59	4	20:05	10
B2	42	4	20:07	2
C2	72	4	20:36	29
B2	71	4	20:36	0
B2	64	4	20:37	1
B2	41	4	20:39	2
A2	68	4	20:52	13
D2	40	4	20:58	6
C2	57	4	21:21	23
A2	67	4	21:38	17
C2	58	4	21:43	5
B2	63	4	21:51	8
D2	74	4	22:07	16
D2	61	4	22:11	4
B2	70	4	22:20	9
A2	76	4	22:25	5
B2	66	4	22:29	4
E2	80	4	22:45	16
A2	55	4	22:57	12
C2	60	4	23:24	27
E2	56	4	23:24	0
A2	79	4	24:27	63
A2	78	4	25:04	37

Table 10b. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
C2	81	4	25:32	28
A2	77	4	26:07	35
A2	104	5	19:45	
A2	96	5	20:48	63
C2	103	5	21:22	34
A2	100	5	21:41	19
C2	94	5	22:05	24
A2	98	5	22:28	23
A2	102	5	22:32	4
A2	95	5	22:34	2
B2	93	5	22:36	2
B2	88	5	22:49	13
A2	91	5	22:55	6
C2	121	5	23:04	9
B2	92	5	23:50	46
A2	84	5	23:44	-6
A2	89	5	23:53	9
D2	90	5	24:07	14
E2	101	5	24:11	4
B2	113	5	24:23	12
B2	99	5	24:28	5
C2	119	5	24:54	26
D2	112	5	25:00	6
A2	83	5	25:02	2
E2	108	5	25:09	7
A2	97	5	25:22	13
A2	86	5	25:27	5
B2	125	5	25:36	9
B2	117	5	25:37	1
C2	87	5	25:38	1
E2	111	5	25:51	13
B2	115	5	25:44	-7
C2	116	5	25:48	4
A2	85	5	25:51	3
B2	120	5	26:12	21
D2	110	5	26:16	4
C2	82	5	26:48	32
B2	124	5	27:36	48
B2	107	5	27:40	4
A2	109	5	27:45	5
A2	123	5	27:53	8

Table 10b. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
B2	118	5	28:04	11
A2	106	5	28:04	0
D2	114	5	28:38	34
A2	122	5	28:48	10
E2	105	5	29:30	42
E2	127	5	29:57	27
A2	126	5	31:49	112
B2	155	6	23:43	
A2	150	6	24:52	69
A2	152	6	25:17	25
D2	145	6	25:42	25
B2	136	6	26:01	19
A2	148	6	26:14	13
D2	154	6	26:44	30
B2	151	6	27:18	34
A2	135	6	27:31	13
B2	144	6	27:38	7
E2	147	6	27:44	6
B2	139	6	28:01	17
C2	149	6	28:01	0
C2	140	6	28:12	11
A2	143	6	28:34	22
A2	134	6	28:35	1
A2	133	6	28:59	24
B2	131	6	28:52	-7
C2	142	6	28:59	7
C2	165	6	29:21	22
A2	146	6	29:24	3
B2	161	6	29:32	8
B2	132	6	29:32	0
A2	153	6	29:48	16
A2	168	6	29:59	11
A2	141	6	30:31	32
C2	137	6	30:51	20
E2	130	6	30:57	6
A2	138	6	31:20	23
B2	163	6	31:28	8
C2	164	6	31:22	-6
A2	158	6	31:35	13
B2	160	6	31:33	-2
A2	129	6	31:48	15

Table 10b. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
B2	166	6	32:13	25
D2	159	6	32:43	30
C2	128	6	32:52	9
B2	162	6	33:00	8
A2	167	6	33:23	23
A2	156	6	34:40	77
B2	157	6	34:57	17
E2	169	6	37:19	142
A2	188	7	29:22	
A2	184	7	29:49	27
A2	179	7	30:33	44
C2	176	7	31:01	28
C2	186	7	31:36	35
A2	178	7	32:14	38
A2	175	7	32:33	19
A2	187	7	32:46	13
A2	182	7	32:47	1
A2	183	7	33:6	19
D2	185	7	33:43	37
B2	174	7	34:07	24
C2	181	7	34:11	4
A2	177	7	34:22	11
B2	171	7	34:40	18
B2	173	7	35:04	24
B2	172	7	35:41	37
B2	192	7	35:51	10
E2	180	7	36:07	16
E2	193	7	36:20	13
A2	191	7	36:34	14
A2	170	7	37:44	70
B2	190	7	37:56	12
C2	189	7	39:51	115
A2	202	8	34:56	
A2	201	8	35:25	29
A2	204	8	35:36	11
B2	197	8	35:55	19
A2	200	8	36:49	54
B2	198	8	38:34	105
A2	199	8	38:43	9
A2	203	8	39:05	22
E2	196	8	39:05	0

Table 10b. (continued)

Series 2 Std	Congener (IUPAC)	Number of Chlorines	Observed DB-1 RT min:sec	Separation from preceding isomer
B2	195	8	40:45	100
A2	194	8	42:16	91
E2	205	8	42:44	28
E2	208	9	41:03	
A2	207	9	41:32	29
E2	206	9	44:52	200
E2	209	10	46:55	

Table 11a. Relative Response Factors of 209 CB congeners

Congener IUPAC (or IUPAC/BZ)	# Chlorines	Relative Response Factors ¹			
		Individual	LOC Mean ²	Std Dev	% rsd
1	1	1.14	1.067	0.064	6.0%
2	1	1.02			
3	1	1.04			
4	2	0.72	0.944	0.099	10.5%
5	2	0.98			
6	2	0.98			
7	2	1.01			
8	2	1.07			
9	2	0.91			
10	2	1.08			
11	2	0.89			
12	2	0.92			
13	2	0.84			
14	2	0.96			
15	2	0.97			
16	3	0.59	0.843	0.098	11.6%
17	3	0.65			
18	3	0.66			
19	3	0.67			
20	3	0.81			
21	3	0.89			
22	3	0.84			
23	3	0.89			
24	3	0.88			
25	3	0.92			
26	3	0.90			
27	3	0.86			
28	3	0.93			
29	3	0.92			
30	3	0.90			
31	3	0.94			
32	3	0.91			
33	3	0.87			
34	3	0.89			
35	3	0.81			
36	3	0.88			
37	3	0.87			
38	3	0.88			
39	3	0.88			
40	4	0.67	1.014	0.143	14.1%
41	4	0.75			
42	4	0.83			
43	4	0.79			

Table 11a. (continued)

Congener IUPAC (or IUPAC/BZ)	# Chlorines	Relative Response Factors¹			
		Individual	LOC Mean²	Std Dev	% rsd
44	4	0.82			
45	4	0.76			
46	4	0.80			
47	4	0.92			
48	4	0.92			
49	4	0.86			
50	4	0.85			
51	4	0.93			
52	4	0.84			
53	4	0.93			
54	4	1.19			
55	4	1.06			
56	4	1.11			
57	4	1.13			
58	4	1.12			
59	4	1.08			
60	4	1.11			
61	4	1.12			
62	4	1.10			
63	4	1.08			
64	4	1.08			
65	4	1.08			
66	4	1.08			
67	4	1.17			
68	4	1.15			
69	4	1.02			
70	4	1.10			
71	4	1.15			
72	4	1.10			
73	4	1.14			
74	4	1.21			
75	4	1.13			
76	4	1.10			
77	4	1.01			
78	4	1.03			
79	4	1.10			
80	4	1.18			
81	4	0.97			
82	5	0.60	0.782	0.106	13.6%
83	5	0.59			
84	5	0.65			
85	5	0.69			
86	5	0.69			
87	5	0.65			
88	5	0.66			
89	5	0.65			

Table 11a. (continued)

Congener IUPAC (or IUPAC/BZ)	# Chlorines	Relative Response Factors¹			
		Individual	LOC Mean²	Std Dev	% rsd
90	5	0.70			
91	5	0.75			
92	5	0.92			
93	5	0.68			
94	5	0.69			
95	5	0.70			
96	5	0.70			
97	5	0.71			
98	5	0.72			
99	5	0.81			
100	5	0.79			
101	5	0.79			
102	5	0.80			
103	5	0.73			
104	5	0.86			
105	5	0.81			
106	5	0.72			
107/108	5	0.75			
108/109	5	0.89			
109/107	5	0.82			
110	5	0.92			
111	5	0.88			
112	5	0.92			
113	5	0.82			
114	5	0.74			
115	5	0.95			
116	5	0.84			
117	5	0.90			
118	5	0.72			
119	5	0.91			
120	5	0.87			
121	5	0.93			
122	5	0.67			
123	5	0.83			
124	5	0.71			
125	5	0.89			
126	5	0.97			
127	5	0.99			
128	6	0.71	0.822	0.109	13.2%
129	6	0.65			
130	6	0.64			
131	6	0.75			
132	6	0.76			
133	6	0.70			
134	6	0.75			
135	6	0.70			

Table 11a. (continued)

Congener IUPAC (or IUPAC/BZ)	# Chlorines	Relative Response Factors¹			
		Individual	LOC Mean²	Std Dev	% rsd
136	6	0.87			
137	6	0.73			
138	6	0.85			
139	6	0.84			
140	6	0.79			
141	6	0.76			
142	6	0.69			
143	6	0.74			
144	6	0.67			
145	6	0.91			
146	6	0.81			
147	6	0.81			
148	6	0.65			
149	6	0.84			
150	6	0.99			
151	6	0.65			
152	6	0.87			
153	6	0.84			
154	6	0.74			
155	6	1.04			
156	6	0.93			
157	6	0.90			
158	6	0.95			
159	6	0.84			
160	6	0.88			
161	6	0.91			
162	6	0.85			
163	6	0.99			
164	6	0.93			
165	6	0.92			
166	6	0.88			
167	6	0.85			
168	6	1.01			
169	6	0.93			
170	7	0.77	1.031	0.188	18.2%
171	7	0.92			
172	7	0.84			
173	7	0.8			
174	7	0.89			
175	7	0.99			
176	7	1.32			
177	7	0.91			
178	7	0.98			
179	7	1.35			
180	7	0.92			
181	7	0.97			

Table 11a. (continued)

Congener IUPAC (or IUPAC/BZ)	# Chlorines	Relative Response Factors¹			
		Individual	LOC Mean²	Std Dev	% rsd
182	7	1.00			
183	7	1.03			
184	7	1.41			
185	7	0.99			
186	7	1.34			
187	7	1.09			
188	7	1.31			
189	7	0.76			
190	7	1.03			
191	7	1.03			
192	7	1.01			
193	7	1.09			
194	8	0.90	1.051	0.200	19.0%
195	8	0.88			
196	8	0.82			
197	8	1.32			
198	8	0.86			
199/201	8	0.91			
200/199	8	1.19			
201/200	8	1.27			
202	8	1.33			
203	8	0.87			
204	8	1.22			
205	8	1.04			
206	9	0.44	0.593	0.142	23.9%
207	9	0.62			
208	9	0.72			
209	10	0.93	0.930		

1. RRF of each congener calculated against the closest eluting ¹³C-labeled congener with same number of chlorine substituents (i.e. LOC).

2. Mean RRF statistics for congeners in that LOC

Table 11b. Summary of congener Relative Response Factors

# of Chlorines	Mean RRF	# Isomers	Std. dev	% Rsd
1	1.07	3	0.06	6.03%
2	0.94	12	0.10	10.49%
3	0.84	24	0.10	11.61%
4	1.01	42	0.14	14.10%
5	0.78	46	0.11	13.58%
6	0.82	42	0.11	13.20%
7	1.03	24	0.19	18.21%
8	1.05	12	0.20	19.05%
9	0.59	3	0.14	23.91%
10	0.93	1		
All congeners	0.91	209	0.13	14.46%

Table 12. Quantities of Aroclor Mixtures taken for Full Congener Analysis

To allow full congener analysis to stay with the linearity limits of 1668, the concentration of most abundant congener in each Aroclor mixture was used to determine quantity of each taken as indicated below.

Aroclor	Most Abundant Congener (MAC)	IUPAC	Wt %	Concentration Aroclor giving 2 µg/mL of MAC	Nominal weight of Aroclor taken per µvial
1221	1		31.10	3.22	125
1232	1		16.40	6.10	250
1016	18		12.30	8.13	500
1242	18		9.20	10.87	500
1248	53		6.22	16.08	500
5442	118		7	14.29	500
1254	118		12.30	8.13	500
5460	118		6	16.67	500
1260	153		8.80	22.73	1000
1262	180		11.20	17.86	1000
1268	180		20	10	500

Table 13. Composition of Aroclor 1254 on SPB-Octyl

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %
CL1-PCB-1	1.2e+06	2.98	y	13:36	0.028	0.01
CL1-PCB-2	*	*	n	NotFnd	*	0.01
CL1-PCB-3	4.9e+05	6.90	n	16:13	0.013	0.01
CL2-PCB-4	1.3e+06	0.45	n	16:32	0.051	0.07
CL2-PCB-10	4.4e+05	0.07	n	16:44	0.013	0.06
CL2-PCB-9	2.7e+05	0.52	n	18:49	0.008	0.06
CL2-PCB-7	6.5e+04	1.24	n	19:00	0.002	0.05
CL2-PCB-6	5.5e+05	0.46	n	19:18	0.016	0.05
CL2-PCB-5	1.2e+05	0.19	n	19:38	0.004	0.06
CL2-PCB-8	9.3e+05	3.25	n	19:48	0.026	0.05
CL2-PCB-14	1.3e+05	0.21	n	21:37	0.004	0.06
CL2-PCB-11	2.2e+05	0.03	n	22:39	0.007	0.06
CL2-PCB-12/13	3.7e+05	0.32	n	22:57	0.013	0.06
CL2-PCB-15	4.5e+05	1.38	y	23:18	0.015	0.06
CL3-PCB-19	4.1e+04	1.37	n	20:09	0.002	0
CL3-PCB-30/18	1.4e+06	1.02	y	22:15	0.051	0
CL3-PCB-17	3.3e+05	0.83	n	22:43	0.015	0
CL3-PCB-27	*	*	n	NotFnd	*	0
CL3-PCB-24	*	*	n	NotFnd	*	0
CL3-PCB-16	2.2e+05	0.15	n	23:14	0.012	0.01
CL3-PCB-32	4.8e+05	1.35	n	23:49	0.016	0
CL3-PCB-34	*	*	n	NotFnd	*	0
CL3-PCB-23	*	*	n	NotFnd	*	0
CL3-PCB-26/29	9.7e+04	7.48	n	25:41	0.003	0
CL3-PCB-25	*	*	n	NotFnd	*	0
CL3-PCB-31	4.0e+06	0.99	y	26:20	0.127	0
CL3-PCB-28/20	1.6e+06	1.13	y	26:38	0.053	0
CL3-PCB-21/33	1.1e+06	1.02	y	26:55	0.034	0
CL3-PCB-22	6.8e+05	1.20	n	27:21	0.023	0
CL3-PCB-36	*	*	n	NotFnd	*	0
CL3-PCB-39	*	*	n	NotFnd	*	0
CL3-PCB-38	*	*	n	NotFnd	*	0.01
CL3-PCB-35	*	*	n	NotFnd	*	0.01
CL3-PCB-37	3.7e+05	0.91	y	31:03	0.015	0.01
CL4-PCB-54	*	*	n	NotFnd	*	0
CL4-PCB-50/53	2.3e+06	0.79	y	26:03	0.103	0
CL4-PCB-45/51	7.8e+05	0.96	n	26:47	0.066	0.01

Table 13 (cont'd) - Aroclor 1254 on Octyl

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %
CL4-PCB-46	3.1e+05	0.47	n	27:08	0.016	0
CL4-PCB-52	1.3e+08	0.75	y	28:39	5.781	0
CL4-PCB-73	*	*	n	NotFnd	*	0
CL4-PCB-43	*	*	n	NotFnd	*	0
CL4-PCB-69/49	2.4e+07	0.75	y	29:11	1.006	0
CL4-PCB-48	1.4e+06	0.67	y	29:31	0.065	0
CL4-PCB-44/47/65	4.8e+07	0.75	y	29:46	2.07	0
CL4-PCB-59/62/75	4.5e+05	0.74	y	30:07	0.016	0
CL4-PCB-42	2.5e+06	0.77	y	30:20	0.118	0
CL4-PCB-41	1.3e+05	0.67	y	30:45	0.007	0
CL4-PCB-40/71	5.7e+06	0.72	y	30:53	0.253	0
CL4-PCB-64	1.7e+07	0.80	y	31:06	0.698	0
CL4-PCB-72	*	*	n	NotFnd	*	0.01
CL4-PCB-68	*	*	n	NotFnd	*	0.01
CL4-PCB-57	*	*	n	NotFnd	*	0.01
CL4-PCB-58	*	*	n	NotFnd	*	0.01
CL4-PCB-67	*	*	n	NotFnd	*	0.01
CL4-PCB-63	1.0e+06	0.80	y	33:28	0.038	0.01
CL4-PCB-61/70/74/76	1.3e+08	0.77	y	33:51	5.853	0.01
CL4-PCB-66	2.6e+07	0.76	y	34:12	0.936	0.01
CL4-PCB-55	*	*	n	NotFnd	*	0.01
CL4-PCB-56	8.9e+06	0.82	y	34:57	0.341	0.01
CL4-PCB-60	4.2e+06	0.82	y	35:10	0.159	0.01
CL4-PCB-80	*	*	n	NotFnd	*	0.01
CL4-PCB-79	1.9e+06	0.84	y	37:14	0.064	0.01
CL4-PCB-78	*	*	n	NotFnd	*	0.01
CL4-PCB-81	*	*	n	NotFnd	*	0.01
CL4-PCB-77	*	*	n	NotFnd	*	0.01
CL5-PCB-104	*	*	n	NotFnd	*	0
CL5-PCB-96	8.7e+05	1.34	y	30:08	0.041	0
CL5-PCB-103	7.2e+05	1.53	y	32:11	0.033	0
CL5-PCB-94	5.3e+05	1.46	y	32:26	0.028	0
CL5-PCB-95	1.4e+08	1.56	y	32:56	7.162	0
CL5-PCB-100/93	*	*	n	NotFnd	*	0
CL5-PCB-102/98	3.8e+06	1.81	n	33:18	0.19	0
CL5-PCB-88/91	2.0e+07	1.61	y	33:51	1.057	0
CL5-PCB-84	4.3e+07	1.59	y	34:07	2.453	0
CL5-PCB-89	9.5e+05	1.62	y	34:38	0.052	0
CL5-PCB-121	*	*	n	NotFnd	*	0

Table 13 (cont'd) - Aroclor 1254 on Octyl

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %
CL5-PCB-92	2.9e+07	1.56	y	35:26	1.508	0
CL5-PCB-113/90/101	1.9e+08	1.56	y	36:03	8.606	0
CL5-PCB-83/99	7.4e+07	1.59	y	36:40	3.686	0
CL5-PCB-112	*	*	n	NotFnd	*	0
CB-108/119/86/97/125/87	8.1e+07	1.56	y	37:22	3.658	0
CL5-PCB-117/116/85	2.4e+07	1.66	y	38:02	1.035	0
CL5-PCB-110/115	2.2e+08	1.57	y	38:12	8.901	0
CL5-PCB-82	1.5e+07	1.53	y	38:34	0.875	0
CL5-PCB-111	*	*	n	NotFnd	*	0
CL5-PCB-120	*	*	n	NotFnd	*	0
CL5-PCB-107/124	6.5e+06	1.50	y	40:39	0.313	0.09
CL5-PCB-109	1.0e+07	1.48	y	40:54	0.468	0.09
CL5-PCB-123	1.9e+06	1.37	y	41:02	0.091	0.09
CL5-PCB-106	*	*	n	NotFnd	*	0.09
CL5-PCB-118	1.5e+08	1.53	y	41:23	7.74	0.1
CL5-PCB-122	1.9e+06	1.42	y	41:46	0.101	0.1
CL5-PCB-114	4.0e+06	1.51	y	41:58	0.187	0.09
CL5-PCB-105	5.7e+07	1.53	y	42:41	2.88	0.1
CL5-PCB-127	*	*	n	NotFnd	*	0.1
CL5-PCB-126	*	*	n	NotFnd	*	0.12
CL6-PCB-155	*	*	n	NotFnd	*	0
CL6-PCB-152	1.6e+05	1.81	n	36:03	0.008	0
CL6-PCB-150	1.3e+05	1.69	n	36:14	0.006	0
CL6-PCB-136	1.7e+07	1.34	y	36:39	0.888	0
CL6-PCB-145	*	*	n	NotFnd	*	0
CL6-PCB-148	*	*	n	NotFnd	*	0
CL6-PCB-151/135	1.9e+07	0.75	n	39:09	2.574	0
CL6-PCB-154	8.5e+05	1.32	y	39:24	0.048	0
CL6-PCB-144	4.8e+06	1.23	y	39:46	0.299	0
CL6-PCB-147/149	7.8e+07	1.25	y	40:10	4.265	0.02
CL6-PCB-134/143	7.9e+06	1.22	y	40:23	0.854	0.04
CL6-PCB-139/140	3.2e+06	1.27	y	40:47	0.169	0.02
CL6-PCB-131	2.5e+06	1.31	y	41:03	0.15	0.02
CL6-PCB-142	*	*	n	NotFnd	*	0.02
CL6-PCB-132	4.3e+07	1.22	y	41:33	2.619	0.02
CL6-PCB-133	1.3e+06	1.24	y	41:59	0.077	0.02
CL6-PCB-165	*	*	n	NotFnd	*	0.02
CL6-PCB-146	1.5e+07	1.25	y	42:41	0.751	0.02
CL6-PCB-161	*	*	n	NotFnd	*	0.02

Table 13 (cont'd) - Aroclor 1254 on Octyl

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %
CL6-PCB-153/168	9.1e+07	1.24	y	43:21	4.318	0.02
CL6-PCB-141	2.0e+07	1.24	y	43:34	1.142	0.02
CL6-PCB-130	7.8e+06	1.27	y	44:01	0.525	0.03
CL6-PCB-137	8.4e+06	1.46	n	44:15	0.513	0.02
CL6-PCB-164	9.8e+06	1.23	y	44:23	0.435	0.02
CL6-PCB-138/163/129/160	1.4e+08	1.24	y	44:43	10.145	0.03
CL6-PCB-158	2.1e+07	1.20	y	45:07	0.934	0.02
CL6-PCB-128/166	2.6e+07	1.24	y	46:05	1.446	0.02
CL6-PCB-159	3.5e+05	1.32	y	47:03	0.017	0.02
CL6-PCB-162	5.6e+05	1.20	y	47:22	0.029	0.02
CL6-PCB-167	6.5e+06	1.23	y	47:53	0.329	0.02
CL6-PCB-156/157	2.2e+07	1.27	y	49:07	1.28	0.04
CL6-PCB-169	*	*	n	NotFnd	*	0.03
CL7-PCB-188	*	*	n	NotFnd	*	0
CL7-PCB-179	2.8e+06	0.88	n	42:20	0.133	0
CL7-PCB-184	*	*	n	NotFnd	*	0
CL7-PCB-176	1.3e+06	0.99	y	43:14	0.064	0
CL7-PCB-186	*	*	n	NotFnd	*	0
CL7-PCB-178	8.0e+05	0.88	n	45:10	0.05	0
CL7-PCB-175	2.9e+05	0.94	y	45:49	0.019	0
CL7-PCB-187	5.1e+06	0.94	y	46:06	0.303	0
CL7-PCB-182	*	*	n	NotFnd	*	0
CL7-PCB-183	4.2e+06	0.88	n	46:45	0.253	0
CL7-PCB-185	4.2e+05	1.18	y	46:53	0.028	0
CL7-PCB-174	6.0e+06	0.88	n	47:03	0.416	0
CL7-PCB-177	*	*	n	NotFnd	*	0
CL7-PCB-181	2.2e+05	0.89	n	47:56	0.015	0
CL7-PCB-171/173	3.0e+06	1.12	y	48:13	0.213	0
CL7-PCB-172	1.3e+06	0.97	y	49:52	0.104	0
CL7-PCB-192	*	*	n	NotFnd	*	0
CL7-PCB-193/180	1.3e+07	0.90	y	50:34	0.816	0
CL7-PCB-191	3.8e+05	0.81	n	50:56	0.025	0
CL7-PCB-170	7.7e+06	0.95	y	51:57	0.661	0
CL7-PCB-190	1.6e+06	0.77	n	52:29	0.092	0
CL7-PCB-189	3.2e+05	0.57	n	55:13	0.026	0.01
CL8-PCB-202	*	*	n	NotFnd	*	0
CL8-PCB-201	*	*	n	NotFnd	*	0
CL8-PCB-204	*	*	n	NotFnd	*	0
CL8-PCB-197	*	*	n	NotFnd	*	0

Table 13 (cont'd) - Aroclor 1254 on Octyl

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %
CL8-PCB-200	*	*	n	NotFnd	*	0
CL8-PCB-198/199	4.2e+05	0.49	n	52:39	0.046	0
CL8-PCB-196	2.1e+05	1.26	n	53:20	0.023	0
CL8-PCB-203	2.0e+05	0.92	y	53:33	0.02	0
CL8-PCB-195	1.9e+05	0.67	n	55:00	0.018	0
CL8-PCB-194	4.4e+05	0.94	y	57:26	0.048	0.01
CL8-PCB-205	*	*	n	NotFnd	*	0.01
CL9-PCB-208	*	*	n	NotFnd	*	0.01
CL9-PCB-207	*	*	n	NotFnd	*	0.01
CL9-PCB-206	*	*	n	NotFnd	*	0.01
CL10-PCB-209	*	*	n	NotFnd	*	0
Homologue Totals						
Cl-1		0.041 %				
Cl-2		0.159 %				
Cl-3		0.351 %				
Cl-4		17.59 %				
Cl-5		51.065 %				
Cl-6		33.821 %				
Cl-7		3.218 %				
Cl-8		0.155 %				
Cl-9		0 %				
Cl-10		0 %				
Total		106.4 %				

1. Name = Congener or co-eluting congeners. Each identified by number of chlorine substituents (LOC) and followed by IUPAC congener #
2. Response is total integrated peak area of the mass chromatograms peaks for the two ions characteristic for that CB.
3. RA = ion relative abundance measured as peak area ratio (M1 /M2) for the characteristic ion mass chromatograms
4. RA OK? = y when detected RA is within $\pm 15\%$ of theoretical ratio
5. Centroid Retention time of congener or congener group in minutes and seconds
6. Concentration of congener ng/100 ng of Aroclor i.e wt%
7. SDL = sample detection limit based on sum of mass channel noise (noise taken as 4 std. Devs. of baseline noise measured typically over the first minute of the scan function)
8. MS Data file PB88_089/s14

Table 14. Composition of Aroclor 1254 on DB-1

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %
CL1-PCB-1	6.9E+05	3.56	y	09:40	0.033	0
CL1-PCB-2	*	*	n	NotFnd	*	0
CL1-PCB-3	2.2E+05	3	y	10:56	0.012	0
CL2-PCB-4/10	7.6E+05	0.32	n	11:39	0.063	0.11
CL2-PCB-7/9	4.1E+05	0.14	n	12:41	0.029	0.09
CL2-PCB-6	1.9E+05	1.02	n	13:05	0.014	0.09
CL2-PCB-8/5	7.3E+05	1.1	n	13:18	0.055	0.1
CL2-PCB-14	2.9E+05	0.03	n	14:04	0.022	0.1
CL2-PCB-11	*	*	n	NotFnd	*	0.1
CL2-PCB-13/12	2.6E+05	0.03	n	15:04	0.021	0.11
CL2-PCB-15	4.3E+05	0.22	n	15:18	0.033	0.1
CL3-PCB-19	*	*	n	NotFnd	*	0.01
CL3-PCB-30	*	*	n	NotFnd	*	0.01
CL3-PCB-18	7.0E+05	1.3	n	15:15	0.061	0.01
CL3-PCB-17	2.3E+05	1.43	n	15:22	0.02	0.01
CL3-PCB-24/27	*	*	n	NotFnd	*	0.01
CL3-PCB-16/32	2.3E+05	1.78	n	16:07	0.02	0.01
CL3-PCB-34/23	*	*	n	NotFnd	*	0.02
CL3-PCB-26	*	*	n	NotFnd	*	0.01
CL3-PCB-29	*	*	n	NotFnd	*	0.01
CL3-PCB-25	*	*	n	NotFnd	*	0.01
CL3-PCB-31/28	1.6E+06	0.84	n	17:36	0.229	0.01
CL3-PCB-20/21/33	3.3E+05	1.52	n	18:08	0.03	0.01
CL3-PCB-22	1.7E+05	1.37	n	18:29	0.014	0.01
CL3-PCB-36	*	*	n	NotFnd	*	0.01
CL3-PCB-39	*	*	n	NotFnd	*	0.01
CL3-PCB-38	*	*	n	NotFnd	*	0.01
CL3-PCB-35	*	*	n	NotFnd	*	0.01
CL3-PCB-37	*	*	n	NotFnd	*	0.01
CL4-PCB-54	*	*	n	NotFnd	*	0.01
CL4-PCB-50	*	*	n	NotFnd	*	0.01
CL4-PCB-53	1.2E+06	0.72	y	18:12	0.171	0.01
CL4-PCB-45	3.2E+05	0.64	n	18:48	0.052	0.01
CL4-PCB-51	*	*	n	NotFnd	*	0.01
CL4-PCB-46	1.3E+05	1.16	n	19:12	0.024	0.01
CL4-PCB-73	*	*	n	NotFnd	*	0.01
CL4-PCB-52/69	6.6E+07	0.76	y	19:39	8.589	0.01

Table 14. (cont'd) Aroclor 1254 on DB-1

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt % Wt %
CL4-PCB-43/49	1.2E+07	0.73	y	19:54	1.939	0.01
CL4-PCB-48/75	7.9E+05	0.77	y	20:10	0.103	0.01
CL4-PCB-47	1.4E+06	0.67	y	20:03	0.214	0.01
CL4-PCB-65/62	*	*	n	NotFnd	*	0.01
CL4-PCB-44	2.0E+07	0.77	y	20:44	3.775	0.01
CL4-PCB-42/59	1.4E+06	0.84	y	20:55	0.212	0.01
CL4-PCB-64/71/41/72	6.5E+06	0.76	y	21:26	1.096	0.01
CL4-PCB-40	6.5E+05	0.78	y	21:50	0.161	0.02
CL4-PCB-68	*	*	n	NotFnd	*	0.01
CL4-PCB-57	*	*	n	NotFnd	*	0.01
CL4-PCB-58	*	*	n	NotFnd	*	0.01
CL4-PCB-67	*	*	n	NotFnd	*	0.02
CL4-PCB-63	*	*	n	NotFnd	*	0.01
CL4-PCB-74/61	6.5E+06	0.79	y	22:60	1.78	0.02
CL4-PCB-70	2.7E+07	0.76	y	23:12	4.56	0.01
CL4-PCB-76/66	6.7E+06	0.92	n	23:22	1.973	0.02
CL4-PCB-55	2.9E+05	0.66	y	23:50	0.051	0.01
CL4-PCB-56	3.2E+06	0.72	y	24:17	0.296	0.01
CL4-PCB-60	3.2E+06	0.72	y	24:17	0.296	0.01
CL4-PCB-80	6.7E+04	0.33	n	23:36	0.011	0.01
CL4-PCB-79	5.6E+05	0.6	n	25:23	0.081	0.01
CL4-PCB-78	1.0E+05	0.35	n	25:59	0.018	0.01
CL4-PCB-81	*	*	n	NotFnd	*	0.01
CL4-PCB-77	*	*	n	NotFnd	*	0.02
CL5-PCB-104	*	*	n	NotFnd	*	0.02
CL5-PCB-96	4.8E+05	1.74	y	21:40	0.05	0.03
CL5-PCB-103	3.6E+05	1.53	y	22:15	0.046	0.03
CL5-PCB-94	3.3E+05	1.34	y	22:57	0.042	0.03
CL5-PCB-98/102/93/95	7.4E+07	1.56	y	23:27	9.53	0.03
CL5-PCB-100	7.0E+04	1.3	n	22:34	0.009	0.03
CL5-PCB-88	*	*	n	NotFnd	*	0.04
CL5-PCB-91	8.4E+06	1.48	y	23:49	1.07	0.03
CL5-PCB-84/92/89	1.9E+07	1.55	y	24:38	8.156	0.1
CL5-PCB-121	*	*	n	NotFnd	*	0.03
CL5-PCB-90/101	1.0E+08	1.57	y	25:06	11.279	0.03
CL5-PCB-113/99	3.3E+07	1.59	y	25:23	5.653	0.04
CL5-PCB-83/112	3.4E+06	1.54	y	25:58	0.413	0.03
CL5-PCB-108	*	*	n	NotFnd	*	0.03
CL5-PCB-119	9.9E+05	1.36	y	25:50	0.102	0.03

Table 14. (cont'd) Aroclor 1254 on DB-1

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %	Wt %
CL5-PCB-86	*	*	n	NotFnd	*	0.04	
CL5-PCB-97	2.1E+07	1.59	y	26:18	2.871	0.03	
CL5-PCB-117/125/87	3.8E+07	1.61	y	26:34	4.195	0.03	
CL5-PCB-115/116/111/85	1.0E+07	1.52	y	26:48	1.134	0.03	
CL5-PCB-82	5.9E+06	1.5	y	27:47	0.969	0.04	
CL5-PCB-120/110	9.7E+07	1.54	y	27:13	10.601	0.03	
CL5-PCB-124/107/109	2.6E+06	1.38	y	28:42	0.633	0.13	
CL5-PCB-123	5.1E+05	1.24	n	28:50	0.091	0.1	
CL5-PCB-118/106	4.5E+07	1.52	y	29:03	7.43	0.09	
CL5-PCB-122	3.2E+05	1.63	y	29:47	0.056	0.09	
CL5-PCB-114	1.3E+06	1.1	n	29:38	0.204	0.09	
CL5-PCB-105	1.5E+07	1.38	y	30:31	3.121	0.12	
CL5-PCB-127	3.5E+04	0.37	n	30:56	0.011	0.21	
CL5-PCB-126	*	*	n	NotFnd	*	0.21	
CL6-PCB-155	*	*	n	NotFnd		0	
CL6-PCB-152	*	*	n	NotFnd		0	
CL6-PCB-150	6.4E+04	1.42	y	25:47	0.008	0	
CL6-PCB-136	9.8E+06	1.21	y	26:58	1.391	0	
CL6-PCB-145	*	*	n	NotFnd		0	
CL6-PCB-148	*	*	n	NotFnd		0	
CL6-PCB-151	5.9E+06	1.26	y	28:17	1.23	0.03	
CL6-PCB-135/144	5.5E+06	1.19	y	28:30	2.08	0.06	
CL6-PCB-154	4.4E+05	1.06	y	27:40	0.08	0	
CL6-PCB-147	1.2E+06	0.98	n	28:43	0.239	0.03	
CL6-PCB-139/149	3.6E+07	1.29	y	28:60	6.804	0.03	
CL6-PCB-134/143	3.0E+06	1.08	y	29:35	0.634	0.03	
CL6-PCB-140	*	*	n	NotFnd		0.03	
CL6-PCB-131	1.0E+06	1.28	y	29:51	0.238	0.04	
CL6-PCB-133/142	4.9E+05	1.15	y	29:58	0.106	0.03	
CL6-PCB-165/146	4.6E+06	1.27	y	30:23	0.883	0.03	
CL6-PCB-132/161	1.9E+07	1.29	y	30:32	3.582	0.03	
CL6-PCB-153	3.3E+07	1.24	y	30:47	6.301	0.03	
CL6-PCB-168	*	*	n	NotFnd		0.03	
CL6-PCB-141	6.7E+06	1.28	y	31:30	1.63	0.04	
CL6-PCB-130	2.7E+06	1.35	y	31:59	0.63	0.04	
CL6-PCB-137	2.4E+06	1.25	y	31:53	0.582	0.04	
CL6-PCB-138/163/164	5.3E+07	1.27	y	32:21	9.337	0.03	
CL6-PCB-129	2.5E+06	1.23	y	32:49	0.621	0.04	
CL6-PCB-158/160	7.1E+06	1.28	y	32:35	1.271	0.03	

Table 14. (cont'd) Aroclor 1254 on DB-1

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt %
CL6-PCB-166	4.1E+05	1.57	n	33:15	0.068	0.03
CL6-PCB-128	7.4E+06	1.09	y	33:54	1.744	0.04
CL6-PCB-159	*	*	n	NotFnd		0.03
CL6-PCB-162	*	*	n	NotFnd		0.03
CL6-PCB-167	1.5E+06	1.52	n	34:26	0.318	0.03
CL6-PCB-156	4.5E+06	1.35	y	35:44	1.068	0.05
CL6-PCB-157	1.1E+06	1.32	y	35:59	0.202	0.04
CL6-PCB-169	*	*	n	NotFnd		0.06
CL7-PCB-188	*	*	n	NotFnd		0.01
CL7-PCB-179	1.3E+06	0.78	n	31:35	0.161	0.01
CL7-PCB-184	*	*	n	NotFnd		0.01
CL7-PCB-176	7.1E+05	1.16	y	32:01	0.095	0.01
CL7-PCB-186	*	*	n	NotFnd		0.01
CL7-PCB-178	3.8E+05	1.19	y	33:16	0.063	0.01
CL7-PCB-175	1.2E+05	1.75	n	33:38	0.022	0.01
CL7-PCB-187/182	2.1E+06	0.99	y	33:48	0.368	0.01
CL7-PCB-183	1.5E+06	0.9	y	34:09	0.271	0.01
CL7-PCB-185	2.2E+05	1.09	y	34:45	0.042	0.01
CL7-PCB-174/181	2.4E+06	0.85	n	35:10	0.455	0.01
CL7-PCB-177	1.5E+06	1.03	y	35:26	0.303	0.01
CL7-PCB-171	9.3E+05	1.08	y	35:45	0.183	0.01
CL7-PCB-173	*	*	n	NotFnd		0.01
CL7-PCB-172	2.9E+05	0.72	n	36:44	0.069	0.01
CL7-PCB-192	*	*	n	NotFnd		0.01
CL7-PCB-193	*	*	n	NotFnd		0.01
CL7-PCB-180	4.1E+06	0.96	y	37:11	0.912	0.01
CL7-PCB-191	6.9E+04	0.75	n	37:37	0.014	0.01
CL7-PCB-170	2.2E+06	0.88	n	38:50	0.555	0.01
CL7-PCB-190	6.5E+05	1.23	n	39:02	0.12	0.01
CL7-PCB-189	*	*	n	NotFnd		0.02
CL8-PCB-202	*	*	n	NotFnd		0.01
CL8-PCB-201	*	*	n	NotFnd		0.01
CL8-PCB-204	*	*	n	NotFnd		0.01
CL8-PCB-197	*	*	n	NotFnd		0.01
CL8-PCB-200	*	*	n	NotFnd		0.01
CL8-PCB-198	*	*	n	NotFnd		0.01
CL8-PCB-199	3.4E+04	2.32	n	39:49	0.011	0.01
CL8-PCB-196/203	1.2E+05	1.02	y	40:10	0.038	0.01
CL8-PCB-195	*	*	n	NotFnd		0.01

Table 14. (cont'd) Aroclor 1254 on DB-1

Name ¹	Response ²	RA ³	RA ⁴ OK?	RT ⁵ min:sec	Conc ⁶ (Wt %)	SDL ⁷ Wt % Wt %
CL8-PCB-194	*	*	n	NotFnd		0.01
CL8-PCB-205	*	*	n	NotFnd		0.01
CL9-PCB-208	*	*	n	NotFnd		0.01
CL9-PCB-207	*	*	n	NotFnd		0.01
CL9-PCB-206	*	*	n	NotFnd		0.01
CL10-PCB-209	*	*	n	NotFnd		0.01
Homologue Totals						
Cl-1	0.045 %					
Cl-2	0.237 %					
Cl-3	0.374 %					
Cl-4	25.402 %					
Cl-5	67.666 %					
Cl-6	41.047 %					
Cl-7	3.633 %					
Cl-8	0.049 %					
Cl-9	0 %					
Cl-10	0 %					
		138.453 %				

1. Name = Congener or co-eluting congeners. Each identified by number of chlorine substituents (LOC) and followed by IUPAC congener #
2. Response is total integrated peak area of the mass chromatograms peaks for the two ions characteristic for that CB. * = peak not found
3. RA = ion relative abundance measured as peak area ratio (M1 /M2) for the characteristic ion mass chromatograms
4. RA OK? = y when detected RA is within $\pm 15\%$ of theoretical ratio
5. Centroid Retention time of congener or congener group in min:sec
6. Concentration of congener ng/100 ng of Aroclor i.e. wt %
7. SDL = sample detection limit based on sum of mass channel noise (noise taken as 4 Std. Devs. of baseline noise measured typically over the first minute of the scan function)
8. MS Data file PB88_090a/s14

Table 15. Wt percent composition of Aroclor 1254 by combination of SPB-Octyl and DB-1 data and comparison to published congener data.

Congener IUPAC#	Reporting ¹ column	Co-eluting isomers	Congener Concn. wt %	SDL ² wt %	RA	RA?	S.P.D. ³	G.Frame ⁴	G.Frame ⁴
							MS data wt %	wt %	ECD data wt %
1	Octyl		0.028	0.01	2.98	y		0.016	
2	Octyl		0	0.01	*	n			
3	Octyl		0.013	0.01	6.90	n		0.001	
4	Octyl		0.051	0.07	0.45	n		0.029	0.549
5	Octyl		0.004	0.06	0.19	n		0.001	
6	Octyl		0.016	0.05	0.46	n		0.011	
7	Octyl		0.002	0.05	1.24	n		0.007	
8	Octyl		0.026	0.05	3.25	n		0.046	0.139
9	Octyl		0.008	0.06	0.52	n		0.006	0.067
10	Octyl		0.013	0.06	0.07	n		0.001	0.171
11	Octyl		0.007	0.06	0.03	n			
12	Octyl	12+13	See 13	0.06	0.32	n		0.002	
13	Octyl	12+13	0.013	0.06	0.32	n		0.017	
14	Octyl		0.004	0.06	0.21	n			
15	Octyl		0.015	0.06	1.38	y		0.013	
16	Octyl		0.012	0.01	0.15	n		0.034	0.069
17	Octyl		0.015	0.00	0.83	n	0.19	0.029	0.089
18	DB-1		0.061	0.01	1.30	n	0.41	0.085	0.169
19	Octyl		0.002	0.00	1.37	n		0.008	
20	Octyl	28+20	See 28	0.00	1.13	y		0.004	
21	Octyl	21+33	See 33	0.00	1.02	y			
22	Octyl		0.023	0.00	1.20	n		0.024	0.056
23	Octyl		0	0.00	*	n			
24	Octyl		0	0.00	*	n			0.028
25	Octyl		0	0.00	*	n		0.005	
26	DB-1		0	0.01	*	n		0.010	0.033
27	Octyl		0	0.00	*	n		0.004	0.060
28	Octyl	28+20	0.053	0.00	1.13	y	0.25	0.062	0.121
29	DB-1		0	0.01	*	n			
30	DB-1		0	0.01	*	n			
31	Octyl		0.127	0.00	0.99	y	0.22	0.115	0.179
32	Octyl		0.016	0.00	1.35	n		0.022	0.162
33	Octyl	21+33	0.034	0.00	1.02	y	0.14	0.050	0.113
34	Octyl		0	0.00	*	n			
35	Octyl		0	0.01	*	n			
36	Octyl		0	0.00	*	n			

Table 15 (continued)
Aroclor 1254 by combination of SPB-Octyl and DB-1 data

Congener IUPAC#	Reporting ¹ column	Co-eluting isomers	Congener Concn. wt %	SDL ² wt %	RA	RA?	S.P.D. ³ wt %	G.Frame ⁴ MS data wt %	G.Frame ⁴ ECD data wt %
37	Octyl		0.015	0.01	0.91	y		0.023	
38	Octyl		0	0.01	*	n			
39	Octyl		0	0.00	*	n			
40	DB-1		0.161	0.02	0.78	y	0.2	0.149	0.257
41	Octyl		0.007	0.00	0.67	y	0.64	0.743	0.019
42	Octyl		0.118	0.00	0.77	y	0.23	0.101	0.167
43	Octyl		0	0.00	*	n			
44	DB-1		3.775	0.01	0.77	y	2.03	0.612	0.875
45	DB-1		0.052	0.01	0.64	n		0.033	0.049
46	Octyl		0.016	0.00	0.47	n		0.014	0.044
47	DB-1		0.214	0.01	0.67	y	0.17	0.070	0.091
48	Octyl		0.065	0.00	0.67	y	0.14	0.059	0.121
49	Octyl	69+49	1.006	0.00	0.75	y	1.64	0.297	0.456
50	DB-1		0	0.01	*	n			
51	DB-1		0	0.01	*	n		0.005	
52	Octyl		5.781	0.00	0.75	y	5.18	0.777	1.135
53	DB-1		0.171	0.01	0.72	y	0.09	0.046	0.118
54	Octyl		0	0.00	*	n			
55	Octyl		0	0.01	*	n		0.006	0.305
56	Octyl		0.341	0.01	0.82	y	0.58	1.186	1.656
57	Octyl		0	0.01	*	n			0.040
58	Octyl		0	0.01	*	n			
59	Octyl	59+62+75	0.016	0.00	0.74	y		0.009	0.033
60	Octyl		0.159	0.01	0.82	y	0.54	0.684	1.143
61	DB-1	74+61	See 74	0.02	0.79	y			
62	DB-1	65+62	0	0.01	*	n			
63	Octyl		0.038	0.01	0.80	y	0.05	0.097	0.157
64	Octyl		0.698	0.00	0.80	y	0.45	0.313	0.602
65	DB-1	65+62	See 62	0.01	*	n			
66	Octyl		0.936	0.01	0.76	y	0.59	3.304	3.725
67	Octyl		0	0.01	*	n	0.09	0.010	0.583
68	Octyl		0	0.01	*	n			
69	Octyl	69+49	See 49	0.00	0.75	y			
70	DB-1		4.56	0.01	0.76	y	3.21	5.692	5.911
71	Octyl	40+71	See 40	0.00	0.72	y		0.092	0.156
72	Octyl		0	0.01	*	n			
73	Octyl		0	0.00	*	n			
74	DB-1	74+61	1.78	0.02	0.79	y	0.78	2.221	2.564
75	Octyl	59+62+75	See 59	0.00	0.74	y			

Table 15 (continued)
Aroclor 1254 by combination of SPB-Octyl and DB-1 data

Congener IUPAC#	Reporting ¹ column	Co-eluting isomers	Congener Concn. wt %	SDL ² wt %	RA	RA?	S.P.D. ³ wt %	G.Frame ⁴ MS data wt %	G.Frame ⁴ ECD data wt %
76	Octyl	61+70+74+76	See 70	0.01	0.77	y		0.006	
77	Octyl		0	0.01	*	n		0.114	0.223
78	Octyl		0	0.01	*	n			0.088
79	Octyl		0.064	0.01	0.84	y			
80	Octyl		0	0.01	*	n			
81	Octyl		0	0.01	*	n			
82	Octyl		0.875	0.00	1.53	y	0.95	1.423	1.814
83	DB-1	83+112	0.413	0.03	1.54	y	0.45	0.227	0.494
84	Octyl		2.453	0.00	1.59	y	1.95	1.327	2.121
85	Octyl	117+116+85	1.035	0.00	1.66	y	1.66	2.280	2.604
86	DB-1		0	0.04	*	n		0.071	
87	Octyl	108+119+86+97+1 25+87	3.556	0.00	1.56	y	3.78	3.201	3.423
88	DB-1		0	0.04	*	n		0.010	
89	Octyl		0.052	0.00	1.62	y		0.062	0.124
90	Octyl	113+90+101	see 101	0.00	1.56	y	0.93	0.124	
91	DB-1		1.07	0.03	1.48	y	0.83	0.502	0.624
92	Octyl		1.508	0.00	1.56	y	1.58	0.503	1.152
93	Octyl	100+93	0	0.00	*	n		0.006	0.110
94	Octyl		0.028	0.00	1.46	y		0.012	
95	Octyl		7.162	0.00	1.56	y	6.02	1.816	2.248
96	Octyl		0.041	0.00	1.34	y	0.08	0.012	0.079
97	DB-1		2.871	0.03	1.59	y	2.55	2.554	3.252
98	Octyl	102+98	see 102	0.00	1.81	n		0.081	
99	Octyl	83+99	3.686	0.00	1.59	y	3.6	3.550	5.041
100	DB-1		0.009	0.03	1.30	n	0.1	0.004	0.081
101	Octyl	113+90+101	8.606	0.00	1.56	y	7.94	4.930	5.277
102	Octyl	102+98	0.19	0.00	1.81	n		0.078	0.133
103	Octyl		0.033	0.00	1.53	y		0.007	0.064
104	Octyl		0	0.00	*	n			
105	Octyl		2.88	0.10	1.53	y	3.83	6.063	6.803
106	Octyl		0	0.09	*	n			
107	Octyl	107+124	see 124	0.09	1.50	y			0.366
108	DB-1		0	0.03	*	n			
109	Octyl		0.468	0.09	1.48	y	0.72	0.638	1.113
110	Octyl	110+115	8.901	0.00	1.57	y	5.85	7.420	7.835
111	Octyl		0	0.00	*	n			
112	Octyl		0	0.00	*	n		0.010	
113	Octyl	113+90+101	see 101	0.00	1.56	y			0.102

Table 15 (continued)
Aroclor 1254 by combination of SPB-Octyl and DB-1 data

Congener IUPAC#	Reporting ¹ column	Co-eluting isomers	Congener Concn.	SDL ²	RA	RA?	S.P.D. ³	G.Frame ⁴	G.Frame ⁴
							wt %	wt %	wt %
114	Octyl		0.187	0.09	1.51	y		0.443	0.606
115	Octyl	110+115	see 110	0.00	1.57	y	0.3	0.321	0.461
116	Octyl	117+116+85	see 85	0.00	1.66	y			
117	Octyl	117+116+85	see 85	0.00	1.66	y		0.123	0.261
118	Octyl		7.74	0.10	1.53	y	6.39	12.273	13.157
119	DB-1		0.102	0.03	1.36	y	0.14	0.136	0.226
120	Octyl		0	0.00	*	n			
121	Octyl		0	0.00	*	n			
122	Octyl		0.101	0.10	1.42	y	0.5	0.196	0.323
123	Octyl		0.091	0.09	1.37	y	0.81	0.262	0.625
124	Octyl	107+124	0.313	0.09	1.50	y		0.376	0.568
125	Octyl	108+119+86+97+1 25+87	see 97	0.00	1.56	y		0.035	
126	Octyl		0	0.12	*	n		0.024	
127	Octyl		0	0.10	*	n			
128	DB-1		1.744	0.04	1.09	y	2.07	1.520	1.740
129	DB-1		0.621	0.04	1.23	y	0.23	0.392	0.495
130	Octyl		0.525	0.03	1.27	y	0.63	0.271	0.478
131	Octyl		0.15	0.02	1.31	y	0.16	0.089	0.104
132	Octyl		2.619	0.02	1.22	y	1.98	1.402	1.725
133	Octyl		0.077	0.02	1.24	y		0.060	0.094
134	Octyl	134+143	0.854	0.04	1.22	y	0.49	0.168	0.322
135	Octyl	151+135	2.574	0.00	0.75	n	1.62	0.286	0.378
136	Octyl		0.888	0.00	1.34	y	1.12	0.242	0.442
137	Octyl		0.513	0.02	1.46	n	0.25	0.447	0.675
138	DB-1	138+163+164	8.902	0.03	1.27	y	3.2	5.156	4.899
139	Octyl	139+140	0.169	0.02	1.27	y		0.057	0.194
140	DB-1		0	0.03	*	n		0.027	
141	Octyl		1.142	0.02	1.24	y	1.04	0.603	0.794
142	Octyl		0	0.02	*	n			0.313
143	Octyl	134+143	see 134	0.04	1.22	y		0.021	0.070
144	Octyl		0.299	0.00	1.23	y		0.095	0.201
145	Octyl		0	0.00	*	n			0.482
146	Octyl		0.751	0.02	1.25	y	0.83	0.429	0.531
147	DB-1		0.239	0.03	0.98	n		0.066	0.142
148	Octyl		0	0.00	*	n			
149	DB-1	139+149	6.727	0.03	1.29	y	2.21	1.718	2.272
150	Octyl		0.006	0.00	1.69	n		0.003	
151	DB-1		1.23	0.03	1.26	y	1.17	0.178	0.353

Table 15 (continued)
Aroclor 1254 by combination of SPB-Octyl and DB-1 data

Congener IUPAC#	Reporting ¹ column	Co-eluting isomers	Congener Concn.	SDL ²	RA	RA?	S.P.D. ³	G.Frame ⁴	G.Frame ⁴
							wt %	wt %	wt %
152	Octyl		0.008	0.00	1.81	n		0.002	0.380
153	DB-1		6.301	0.03	1.24	y	4.26	3.068	3.470
154	Octyl		0.048	0.00	1.32	y		0.030	
155	Octyl		0	0.00	*	n			
156	DB-1		1.068	0.05	1.35	y	1.62	0.993	1.252
157	DB-1		0.202	0.04	1.32	y		0.216	0.325
158	Octyl		0.934	0.02	1.20	y	0.77	0.732	1.057
159	Octyl		0.017	0.02	1.32	y			
160	DB-1	158+160	0.337	0.03	1.28	y			
161	Octyl		0	0.02	*	n			
162	Octyl		0.029	0.02	1.20	y		0.025	0.068
163	Octyl	138+163+129+160	see 138	0.03	1.24	y		0.835	0.645
164	Octyl		0.435	0.02	1.23	y		0.193	0.398
165	Octyl		0	0.02	*	n			
166	DB-1		0.068	0.03	1.57	n		0.047	0.154
167	Octyl		0.329	0.02	1.23	y	0.21	0.289	0.410
168	DB-1		0.068	0.03	1.57	n		0.005	
169	Octyl		0	0.03	*	n			
170	Octyl		0.661	0.00	0.95	y	0.31	0.296	0.427
171	DB-1		0.183	0.01	1.08	y	0.5	0.068	0.116
172	Octyl		0.104	0.00	0.97	y	0.05	0.028	0.058
173	DB-1		0	0.01	*	n	0.09		
174	Octyl		0.416	0.00	0.88	n	0.34	0.112	0.226
175	Octyl		0.019	0.00	0.94	y	0.05		0.028
176	Octyl		0.064	0.00	0.99	y	0.32	0.013	0.578
177	Octyl		0	0.00	*	n	0.21	0.065	0.127
178	Octyl		0.05	0.00	0.88	n	1.35	0.024	0.859
179	Octyl		0.133	0.00	0.88	n	0.21	0.023	0.154
180	DB-1		0.912	0.01	0.96	y	0.38	0.364	0.516
181	Octyl		0.015	0.00	0.89	n			
182	Octyl		0	0.00	*	n			
183	Octyl		0.253	0.00	0.88	n	0.17	0.080	0.190
184	Octyl		0	0.00	*	n			
185	Octyl		0.028	0.00	1.18	y		0.011	0.015
186	Octyl		0	0.00	*	n			
187	Octyl		0.303	0.00	0.94	y	0.32	0.069	0.239
188	Octyl		0	0.00	*	n			
189	Octyl		0.026	0.01	0.57	n		0.012	0.034
190	Octyl		0.092	0.00	0.77	n	0.08	0.043	0.090
191	Octyl		0.025	0.00	0.81	n		0.027	

Table 15 (continued)
Aroclor 1254 by combination of SPB-Octyl and DB-1 data

Congener IUPAC#	Reporting ¹ column	Co-eluting isomers	Congener Concn. wt %	SDL ² wt %	RA	RA?	S.P.D. ³ wt %	G.Frame ⁴ MS data wt %	G.Frame ⁴ ECD data wt %
192	Octyl		0	0.00	*	n			
193	DB-1		0	0.01	*	n			0.037
194	Octyl		0.048	0.01	0.94	y		0.008	0.046
195	Octyl		0.018	0.00	0.67	n			0.032
196	Octyl		0.023	0.00	1.26	n			0.019
197	Octyl		0	0.00	*	n			
198	DB-1		0	0.01	*	n			
199	DB-1		0.011	0.01	2.32	n		0.010	0.024
200	Octyl		0	0.00	*	n			
201	Octyl		0	0.00	*	n	0.68		
202	Octyl		0	0.00	*	n			0.528
203	Octyl		0.02	0.00	0.92	y		0.009	0.016
204	Octyl		0	0.00	*	n			
205	Octyl		0	0.01	*	n			
206	Octyl		0	0.01	*	n		0.042	0.088
207	Octyl		0	0.01	*	n			0.009
208	Octyl		0	0.01	*	n		0.020	0.040
209	Octyl		0	0.00	*	n			

Homologue Totals

Cl-1	0.041 wt %
Cl-2	0.159 wt %
Cl-3	0.358 wt %
Cl-4	19.958 wt %
Cl-5	54.371 wt %
Cl-6	39.874 wt %
Cl-7	3.284 wt %
Cl-8	0.12 wt %
Cl-9	0 wt %
Cl-10	0 wt %

118.17 wt %

23 incompletely resolved components, reported at the most abundant isomer
 21 minor congeners co-eluting as components in these GC peaks

44 congeners reported from 23 incompletely resolved peaks

Table 15 (continued)
Aroclor 1254 by combination of SPB-Octyl and DB-1 data

- 1 Column type selected to report congener
- 2 SDL = sample detection limit.
- 3 S.P.D. = Data for this Aroclor reported by Schultz, Petrick and Duinker (1989) E.S & T 23:852-859.
- 4 G.Frame =

Table 16. Labeled PCBs CBs in expanded version Method 1668 and Method 1668 Rev A

Full Congener 1668 Labeled PCB Congener	IUPAC	Full congener 1668, Rev A Labeled PCB Congener	IUPAC
Surrogates			
$^{13}\text{C}_{12}\text{-4-CB}$	3 L	$^{13}\text{C}_{12}\text{-2-CB}$	1L
$^{13}\text{C}_{12}\text{-4,4'-DiCB}$	15L	$^{13}\text{C}_{12}\text{-4-CB}$	3L
$^{13}\text{C}_{12}\text{-2,4,4'-TrCB}$	28L	$^{13}\text{C}_{12}\text{-2,2'-DiCB}$	4L
$^{13}\text{C}_{12}\text{-3,3',4,4'-TeCB}$	77L	$^{13}\text{C}_{12}\text{-4,4'-DiCB}$	15L
$^{13}\text{C}_{12}\text{-2,3,3',4,4'-PeCB}$	105L	$^{13}\text{C}_{12}\text{-2,2'6'-TrCB}$	19L
$^{13}\text{C}_{12}\text{-2,3',4,4',5-PeCB}$	118L	$^{13}\text{C}_{12}\text{-2,4,4'-TrCB}$	37L
$^{13}\text{C}_{12}\text{-3,3',4,4',5-PeCB}$	126L	$^{13}\text{C}_{12}\text{-2,2',6,6'-TeCB}$	54L
$^{13}\text{C}_{12}\text{-2,3,3',4,4',5-HxCB}$	156L	$^{13}\text{C}_{12}\text{-3,3',4,4'-TeCB}$	77L
$^{13}\text{C}_{12}\text{-2,3,3',4,4',5'-HxCB}$	157L	$^{13}\text{C}_{12}\text{-3,4,4',5'-TeCB}$	81L
$^{13}\text{C}_{12}\text{-3,3',4,4',5,5'-HxCB}$	169L	$^{13}\text{C}_{12}\text{-2,2',4,6,6'-PeCB}$	104L
$^{13}\text{C}_{12}\text{-2,2',3,4,4',5,5'-HpCB}$	180L	$^{13}\text{C}_{12}\text{-2,3,3',4,4'-PeCB}$	105L
$^{13}\text{C}_{12}\text{-2,3,3',4,4',5,5'-HpCB}$	189L	$^{13}\text{C}_{12}\text{-2,3,4,4',5-PeCB}$	114L
$^{13}\text{C}_{12}\text{-2,2',3,3',4,4',5,5'-OcCB}$	194L	$^{13}\text{C}_{12}\text{-2,3',4,4',5-PeCB}$	118L
$^{13}\text{C}_{12}\text{-2,2',3,3',4,5,5,6,6'-NCB}$	208L	$^{13}\text{C}_{12}\text{-2',3,4,4',5-PeCB}$	123L
$^{13}\text{C}_{12}\text{-Deca-CB}$	209L	$^{13}\text{C}_{12}\text{-3,3',4,4',5-PeCB}$	126L
		$^{13}\text{C}_{12}\text{-2,2,4,4,6,6'-HxCB}$	155L
		$^{13}\text{C}_{12}\text{-2,3,3',4,4',5-HxCB}$	156L
		$^{13}\text{C}_{12}\text{-2,3,3',4,4',5'-HxCB}$	157L
		$^{13}\text{C}_{12}\text{-3,3',4,4',5,5'-HxCB}$	169L
		$^{13}\text{C}_{12}\text{-2,2',3,4',5,6,6'-HpCB}$	188L
		$^{13}\text{C}_{12}\text{-2,3,3',4,4',5,5'-HpCB}$	189L
		$^{13}\text{C}_{12}\text{-2,2',3,3',5,5,6,6'-OcCB}$	202L
		$^{13}\text{C}_{12}\text{-2,,3,3',4,4',5,5,6-OcCB}$	205L
		$^{13}\text{C}_{12}\text{-2,2',3,3',4,4',5,5',6-NoCB}$	206L
		$^{13}\text{C}_{12}\text{-2,2',3,3',4,4',5,5,6,6'-NoCB}$	208L
		$^{13}\text{C}_{12}\text{-DecaCB}$	209L
Clean-up Standards			
$^{13}\text{C}_{12}\text{-3,4,4',5-TCB}$	81L	$^{13}\text{C}_{12}\text{-2,4,4'-TCB}$	28L
$^{13}\text{C}_{12}\text{-2,3,3',5,5'-PeCB}$	111L	$^{13}\text{C}_{12}\text{-2,3,3',5,5'-PeCB}$	111L
		$^{13}\text{C}_{12}\text{-2,2',3,3',5,5',6,-HpCB}$	178L
Internal Standards			
$^{13}\text{C}_{12}\text{-2,3,3',4,4'-TCB}$	52L	$^{13}\text{C}_{12}\text{-2,5-TCB}$	9L
$^{13}\text{C}_{12}\text{-2,3,3',4,4'-TCB}$	101L	$^{13}\text{C}_{12}\text{-2,2',5,5'-TCB}$	52L
$^{13}\text{C}_{12}\text{-2,3,3',4,4'-TCB}$	138L	$^{13}\text{C}_{12}\text{-2,3,3',4,4'-TCB}$	101L
$^{13}\text{C}_{12}\text{-2,3,3',4,4'-TCB}$	178L	$^{13}\text{C}_{12}\text{-2,3,3',4,4'-TCB}$	138L
		$^{13}\text{C}_{12}\text{-2,3,3',4,4'-TCB}$	178L

Table 17. Concentrations of CB congeners in calibration and calibration verification (VER) standards for method 1668 Rev A

CB Congener	IUPAC ¹	Solution Concentration (ng/mL)					CS-5
		CS-0.2 (Hi sens) ²	CS-1	CS-2	CS-3 (VER)	CS-4	
Native Toxic/LOC							
2-CB	1	0.2	1	5	50	400	2000
4-CB	3	0.2	1	5	50	400	2000
2,2'-DiCB	4	0.2	1	5	50	400	2000
4,4'-DiCB	15	0.2	1	5	50	400	2000
2,2',6'-TrCB	19	0.2	1	5	50	400	2000
2,4,4'-TrCB	37	0.2	1	5	50	400	2000
2,2',6,6'-TeCB	54	0.2	1	5	50	400	2000
3,3',4,4'-TeCB	77	0.2	1	5	50	400	2000
3,4,4',5'-TeCB	81	0.2	1	5	50	400	2000
2,2',4,6,6'-PeCB	104	0.2	1	5	50	400	2000
2,3,3',4,4'-PeCB	105	0.2	1	5	50	400	2000
2,3,4,4',5-PeCB	114	0.2	1	5	50	400	2000
2,3',4,4',5-PeCB	118	0.2	1	5	50	400	2000
2',3,4,4',5-PeCB	123	0.2	1	5	50	400	2000
3,3',4,4',5-PeCB	126	0.2	1	5	50	400	2000
2,2,4,4,6,6'-HxCB	155	0.2	1	5	50	400	2000
2,3,3',4,4',5-HxCB	156	0.2	1	5	50	400	2000
2,3,3',4,4',5'-HxCB	157	0.2	1	5	50	400	2000
3,3',4,4',5,5'-HxCB	169	0.2	1	5	50	400	2000
2,2',3,4',5,6,6'-HpCB	188	0.2	1	5	50	400	2000
2,3,3',4,4',5,5'-HpCB	189	0.2	1	5	50	400	2000
2,2',3,3',5,5,6,6'-OcCB	202	0.2	1	5	50	400	2000
2,3,3',4,4',5,5,6-OcCB	205	0.2	1	5	50	400	2000
2,2',3,3',4,4',5,5,6'-NoCB	206	0.2	1	5	50	400	2000
2,2',3,3',4',5,5,6,6'-NoCB	208	0.2	1	5	50	400	2000
DeCB	209	0.2	1	5	50	400	2000
Labeled toxic/LOC							
13C12-2-CB	1L	100	100	100	100	100	100
13C12-4-CB	3L	100	100	100	100	100	100
13C12-2,2'-DiCB	4L	100	100	100	100	100	100
13C12-4,4'-DiCB	15L	100	100	100	100	100	100
13C12-2,2',6'-TrCB	19L	100	100	100	100	100	100
13C12-2,4,4'-TrCB	37L	100	100	100	100	100	100
13C12-2,2',6,6'-TeCB	54L	100	100	100	100	100	100
13C12-3,3',4,4'-TeCB	77L	100	100	100	100	100	100
13C12-3,4,4',5'-TeCB	81L	100	100	100	100	100	100
13C12-2,2',4,6,6'-PeCB	104L	100	100	100	100	100	100
13C12-2,3,3',4,4'-PeCB	105L	100	100	100	100	100	100
13C12-2,3,4,4',5-PeCB	114L	100	100	100	100	100	100
13C12-2,3',4,4',5-PeCB	118L	100	100	100	100	100	100

Table 17. (continued) Concentrations of CB congeners in calibration and calibration verification (VER) standards for method 1668 Rev A

CB Congener	IUPAC ¹	Solution Concentration (ng/mL)					
		CS-0.2 (Hi sens) ²	CS-1	CS-2	CS-3 (VER)	CS-4	CS-5
Native Toxic/LOC							
13C12-2',3,4,4',5-PeCB	123L	100	100	100	100	100	100
13C12-3,3',4,4',5-PeCB	126L	100	100	100	100	100	100
13C12-2,2,4,4,6,6'-HxCB	155L	100	100	100	100	100	100
13C12-2,3,3',4,4',5-HxCB	156L	100	100	100	100	100	100
13C12-2,3,3',4,4',5'-HxCB	157L	100	100	100	100	100	100
13C12-3,3',4,4',5,5'-HxCB	169L	100	100	100	100	100	100
13C12-2,2',3,4',5,6,6'-HpCB	188L	100	100	100	100	100	100
13C12-2,3,3',4,4',5,5'-HpCB	189L	100	100	100	100	100	100
13C12-2,2',3,3',5,5,6,6'-OcCB	202L	100	100	100	100	100	100
13C12-2,3,3',4,4',5,5,6-OcCB	205L	100	100	100	100	100	100
13C12-2,2',3,3',4,4',5,5',6-NoCB	206L	100	100	100	100	100	100
13C12-2,2',3,3',4',5,5,6,6'-NoCB	208L	100	100	100	100	100	100
13C12-DeCB	209L	100	100	100	100	100	100
Labeled cleanup standard							
13C12-2,4,4'-TCB	28L	100	100	100	100	100	100
13C12-2,3,3',5,5'-PeCB	111L	100	100	100	100	100	100
13C12-2,2',3,3',5,5',6,-HpCB	178L	100	100	100	100	100	100
labeled Injection Internal							
13C12-2,5-DiCB	9L	100	100	100	100	100	100
13C12-2,2',5,5'-TeCB	52L	100	100	100	100	100	100
13C12-2,3,3',4,4'-PeCB	101L	100	100	100	100	100	100
13C12-2,3,3',4,4'-HxCB	138L	100	100	100	100	100	100
13C12-2,3,3',4,4'-HxCB	178L	100	100	100	100	100	100

1. Suffix “l” indicates labeled compound
2. CS-0.2 is an additional low concentration standard used to extend the linearity range for high sensitivity HRGC/HRMS systems

Table 18. Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EMDLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

# Cls	IUPAC #	RT REFERENCE (6)	RT (8)	RRT	RRT LIMITS (1)	Window (7) (seconds)	QUAN REFERENCE	Detection Limits and minimum levels					
								Matrix and concentration (3)		Extract (pg/uL)			
								Water	Other (ng/kg)				
Compounds using 9L (13C12-2,5-DiCB) as Internal Standard													
NATIVE ANALYTES													
Monochlorobiphenyls													
1	1	1L	13:44	1.0012	0.9951 - 1.0073	10	1L	82	260	8	26		13
1	2	3L	16:08	0.9878	0.9847 - 0.9908	6	1L/3L	4	14	0.4	1		1
1	3	3L	16:21	1.0010	0.9980 - 1.0041	6	3L	88	280	9	28		14
Dichlorobiphenyls													
2	4	4L	16:40	1.0010	0.9960 - 1.0060	10	4L	172	547	17	55		27
2	10	4L	16:53	1.0140	1.0110 - 1.0170	6	4L/15L	22	70	2	7		3
2	9	4L	18:55	1.1361	1.1331 - 1.1391	6	4L/15L	20	63	2	6		3
2	7	4L	19:07	1.1481	1.1451 - 1.1512	6	4L/15L	15	49	2	5		2
2	6	4L	19:26	1.1672	1.1642 - 1.1702	6	4L/15L	13	42	1	4		2
2	5	4L	19:48	1.1892	1.1862 - 1.1922	6	4L/15L	11	35	1	3		2
2	8	4L	19:56	1.1972	1.1942 - 1.2002	6	4L/15L	121	384	12	38		19
2	14	15L	21:42	0.9267	0.9246 - 0.9288	6	4L/15L	31	97	3	10		5
2	11	15L	22:42	0.9694	0.9673 - 0.9715	6	4L/15L	105	334	10	33		17
2	13	15L	23:03	0.9843	0.9822 - 0.9865	6	4L/15L	26	84	3	8		4
2	12	15L	23:06	0.9865	0.9843 - 0.9886	6	4L/15L	28	90	3	9		5
2	13/12	15L	23:04	0.9851	0.9829 - 0.9872	6	4L/15L	28	89	3	9		4
2	15	15L	23:26	1.0007	0.9972 - 1.0043	10	15L	183	582	18	58		29
Trichlorobiphenyls													
3	19	19L	20:19	1.0008	0.9967 - 1.0049	10	19L	42	132	4	13		7
3	30	19L	22:15	1.0961	1.0936 - 1.0985	6	19L/37L						
3	18	19L	22:23	1.1026	1.1002 - 1.1051	6	19L/37L						
3	30/18	19L	22:19	1.0993	1.0969 - 1.1018	6	19L/37L	175	556	17	56		28
3	17	19L	22:49	1.1240	1.1215 - 1.1264	6	19L/37L	86	272	9	27		14
3	27	19L	23:06	1.1379	1.1355 - 1.1404	6	19L/37L	59	188	6	19		9

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EDMLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

3	24	19L	23:14	1.1445	1.1420 - 1.1470	6	19L/37L	53	167	5	17	8
3	16	19L	23:25	1.1535	1.1511 - 1.1560	6	19L/37L	35	111	4	11	6
3	32	19L	24:57	1.2291	1.2266 - 1.2315	6	19L/37L	84	266	8	27	13
3	34	19L	25:17	1.2455	1.2430 - 1.2479	6	19L/37L	74	237	7	24	12
3	23	19L	25:26	1.2529	1.2504 - 1.2553	6	19L/37L	50	160	5	16	8
3	29	19L	25:47	1.2701	1.2660 - 1.2742	10	19L/37L					
3	26	19L	25:48	1.2709	1.2668 - 1.2750	10	19L/37L					
3	26/29	19L	25:48	1.2709	1.2668 - 1.2750	10	19L/37L	83	264	8	26	13
3	25	37L	26:04	0.8364	0.8348 - 0.8380	6	19L/37L	55	174	5	17	9
3	31	37L	26:25	0.8476	0.8460 - 0.8492	6	19L/37L	152	484	15	48	24
3	28	37L	26:44	0.8578	0.8551 - 0.8604	10	19L/37L					
3	20	37L	26:49	0.8604	0.8578 - 0.8631	10	19L/37L					
3	28/20	37L	26:47	0.8594	0.8567 - 0.8620	10	19L/37L	192	610	19	61	30
3	21	37L	26:58	0.8652	0.8626 - 0.8679	10	19L/37L	24	76	2	8	4
3	33	37L	27:01	0.8668	0.8642 - 0.8695	10	19L/37L					
3	21/33	37L	26:59	0.8658	0.8631 - 0.8684	10	19L/37L	51	162	5	16	8
3	22	37L	27:29	0.8818	0.8802 - 0.8834	6	19L/37L	90	287	9	29	14
3	36	37L	29:05	0.9332	0.9316 - 0.9348	6	19L/37L	79	251	8	25	13
3	39	37L	29:30	0.9465	0.9449 - 0.9481	6	19L/37L	85	271	9	27	14
3	38	37L	30:10	0.9679	0.9663 - 0.9695	6	19L/37L	83	265	8	26	13
3	35	37L	30:42	0.9850	0.9834 - 0.9866	6	19L/37L	77	244	8	24	12
3	37	37L	31:11	1.0005	0.9989 - 1.0021	6	37L	132	419	13	42	21

LABELLED COMPOUNDS

IUPAC #				RRT QC LIMITS (1)		IUPAC # (2)
1	1L	9L	13:43	0.7257	0.7125 - 0.7390	30
1	3L	9L	16:20	0.8642	0.8510 - 0.8774	30
2	4L	9L	16:39	0.8810	0.8677 - 0.8942	30
2	15L	9L	23:25	1.2390	1.2302 - 1.2478	20
3	19L	9L	20:118	1.0741	1.0608 - 1.0873	30
3	37L	52L	31:10	1.0803	1.0716 - 1.0890	30
					52L	

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EMDLs), and Estimated Minimum Levels (EMLs)
for the 209 PCB congeners on SPB-Octyl.

Compounds using 52L (13C12-2,2',5,5'-TeCB) as Internal Standard													
NATIVE ANALYTES			Tetrachlorobiphenyls										
4	54	54L	23:51	1.0007	0.9972 - 1.0042	10	54L	118	376	12	38		19
4	50	54L	26:07	1.0958	1.0923 - 1.0993	10	54L/81L/77L						
4	53	54L	26:09	1.0972	1.0937 - 1.1007	10	54L/81L/77L						
4	50/53	54L	26:08	1.0965	1.0930 - 1.1000	10	54L/81L/77L	58	186	6	19		9
4	45	54L	26:55	1.1294	1.1259 - 1.1329	10	54L/81L/77L						
4	51	54L	26:58	1.1315	1.1280 - 1.1350	10	54L/81L/77L						
4	45/51	54L	26:57	1.1308	1.1273 - 1.1343	10	54L/81L/77L	51	162	5	16		8
4	46	54L	27:18	1.1455	1.1434 - 1.1476	6	54L/81L/77L	101	320	10	32		16
4	52	54L	28:45	1.2063	1.2042 - 1.2084	6	54L/81L/77L	191	606	19	61		30
4	73	54L	28:52	1.2112	1.2091 - 1.2133	6	54L/81L/77L	160	508	16	51		25
4	43	54L	28:58	1.2154	1.2133 - 1.2175	6	54L/81L/77L	94	299	9	30		15
4	69	54L	29:08	1.2224	1.2189 - 1.2259	10	54L/81L/77L						
4	49	54L	29:16	1.2280	1.2245 - 1.2315	10	54L/81L/77L						
4	69/49	54L	29:12	1.2252	1.2217 - 1.2287	10	54L/81L/77L	115	364	11	36		18
4	48	54L	29:33	1.2399	1.2378 - 1.2420	6	54L/81L/77L	76	240	8	24		12
4	65	54L	29:49	1.2510	1.2476 - 1.2545	10	54L/81L/77L						
4	47	54L	29:50	1.2517	1.2483 - 1.2552	10	54L/81L/77L						
4	44	54L	29:53	1.2538	1.2503 - 1.2573	10	54L/81L/77L						
4	44/47/65	54L	29:50	1.2517	1.2483 - 1.2552	10	54L/81L/77L	195	620	19	62		31
4	62	54L	30:06	1.2629	1.2594 - 1.2664	10	54L/81L/77L						
4	75	54L	30:08	1.2643	1.2608 - 1.2678	10	54L/81L/77L						
4	59	54L	30:12	1.2671	1.2636 - 1.2706	10	54L/81L/77L						
4	59/62/75	54L	30:09	1.2650	1.2615 - 1.2685	10	54L/81L/77L	57	182	6	18		9
4	42	54L	30:26	1.2769	1.2748 - 1.2790	6	54L/81L/77L	61	193	6	19		10
4	41	54L	30:52	1.2951	1.2916 - 1.2986	10	54L/81L/77L						
4	71	54L	30:58	1.2993	1.2958 - 1.3028	10	54L/81L/77L						
4	40	54L	30:01	1.2594	1.2559 - 1.2629	10	54L/81L/77L						
4	41/40/71	54L	30:58	1.2993	1.2958 - 1.3028	10	54L/81L/77L	119	377	12	38		19

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EDMLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

4	64	54L	31:12	1.3091	1.3070 - 1.3112	6	54L/81L/77L	70	221	7	22	11
4	72	81L	31:59	0.8336	0.8323 - 0.8349	6	54L/81L/77L	158	501	16	50	25
4	68	81L	32:18	0.8419	0.8406 - 0.8432	6	54L/81L/77L	149	473	15	47	24
4	57	81L	32:46	0.8540	0.8527 - 0.8553	6	54L/81L/77L	125	397	12	40	20
4	58	81L	33:05	0.8623	0.8610 - 0.8636	6	54L/81L/77L	127	404	13	40	20
4	67	81L	33:13	0.8658	0.8645 - 0.8671	6	54L/81L/77L	147	466	15	47	23
4	63	81L	33:30	0.8732	0.8719 - 0.8745	6	54L/81L/77L	138	439	14	44	22
4	61	81L	33:46	0.8801	0.8775 - 0.8827	12	54L/81L/77L					
4	70	81L	33:53	0.8831	0.8805 - 0.8858	12	54L/81L/77L					
4	76	81L	33:55	0.8840	0.8814 - 0.8866	12	54L/81L/77L					
4	74	54L	33:57	0.8849	0.8827 - 0.8871	10	54L/81L/77L					
4	61/70/74/7	81L	33:55	0.8840	0.8814 - 0.8866	12	54L/81L/77L	171	544	17	54	27
4	66	81L	34:15	0.8927	0.8914 - 0.8940	6	54L/81L/77L	162	515	16	52	26
4	55	81L	34:28	0.8983	0.8970 - 0.8997	6	54L/81L/77L	120	383	12	38	19
4	56	81L	35:03	0.9136	0.9123 - 0.9149	6	54L/81L/77L	98	311	10	31	16
4	60	81L	35:16	0.9192	0.9179 - 0.9205	6	54L/81L/77L	131	418	13	42	21
4	80	81L	35:32	0.9262	0.9248 - 0.9275	6	54L/81L/77L	175	557	18	56	28
4	79	81L	37:16	0.9713	0.9700 - 0.9726	6	54L/81L/77L	173	550	17	55	27
4	78	81L	37:52	0.9870	0.9857 - 0.9883	6	54L/81L/77L	171	543	17	54	27
4	81	81L	38:23	1.0004	0.9991 - 1.0017	6	81L	177	564	18	56	28
4	77	77L	39:02	1.0004	0.9991 - 1.0017	6	77L	169	536	17	54	27

LABELLED COMPOUNDS

IUPAC #	RRT QC LIMITS (1)			IUPAC # (2)
4 54L	52L	23:50	0.8261	0.8203 - 0.8319
4 81L	52L	38:22	1.3299	1.3241 - 1.3356
4 77L	52L	39:01	1.3524	1.3466 - 1.3582

Compounds using 101L (13C12-22'455'-PeCB) as Internal Standard

IUPAC #	RT REFERENCE (6)	RT (8)	RRT	RRT QC LIMITS (1)	Window (7)	QUAN
NATIVE ANALYTES						
Pentachlorobiphenyls						

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EDMLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

5	104	104L	29:46	1.0000	0.9972 - 1.0028	10	104L	228	724	23	72	36
5	96	104L	30:17	1.0174	1.0146 - 1.0202	10	104L/123L/114L/	210	668	21	67	33
5	103	104L	32:11	1.0812	1.0795 - 1.0829	6	104L/123L/114L/	225	717	23	72	36
5	94	104L	32:29	1.0913	1.0896 - 1.0929	6	104L/123L/114L/	121	384	12	38	19
5	95	104L	33:00	1.1086	1.1058 - 1.1114	10	104L/123L/114L/					
5	100	104L	33:06	1.1120	1.1092 - 1.1148	10	104L/123L/114L/					
5	93	104L	33:14	1.1165	1.1137 - 1.1193	10	104L/123L/114L/					
5	102	104L	33:21	1.1204	1.1176 - 1.1232	10	104L/123L/114L/					
5	98	104L	33:26	1.1232	1.1204 - 1.1260	10	104L/123L/114L/					
5	95/100/93/	104L	33:13	1.1159	1.1131 - 1.1187	15	104L/123L/114L/	221	704	22	70	35
5	88	104L	33:48	1.1355	1.1321 - 1.1389	12	104L/123L/114L/					
5	91	104L	33:55	1.1394	1.1366 - 1.1422	10	104L/123L/114L/					
5	88/91	104L	33:52	1.1377	1.1344 - 1.1411	12	104L/123L/114L/	118	375	12	37	19
5	84	104L	34:14	1.1501	1.1484 - 1.1517	6	104L/123L/114L/	124	395	12	39	20
5	89	104L	34:44	1.1669	1.1652 - 1.1685	6	104L/123L/114L/	195	620	19	62	31
5	121	104L	34:57	1.1741	1.1725 - 1.1758	6	104L/123L/114L/	209	664	21	66	33
5	92	123L	35:26	0.8639	0.8627 - 0.8651	6	104L/123L/114L/	115	366	12	37	18
5	113	104L	36:01	0.8781	0.8761 - 0.8801	10	104L/123L/114L/					
5	90	104L	36:03	0.8789	0.8769 - 0.8809	10	104L/123L/114L/					
5	101	104L	36:04	0.8793	0.8773 - 0.8813	10	104L/123L/114L/					
5	113/90/10	104L	36:03	0.8789	0.8769 - 0.8809	10	104L/123L/114L/	241	766	24	77	38
5	83	104L	36:39	0.8935	0.8911 - 0.8960	12	104L/123L/114L/					
5	99	104L	36:41	0.8944	0.8923 - 0.8964	10	104L/123L/114L/					
5	83/99	104L	36:40	0.8939	0.8915 - 0.8964	12	104L/123L/114L/	217	689	22	69	34
5	112	104L	36:51	0.8984	0.8972 - 0.8996	6	104L/123L/114L/	245	780	25	78	39
5	119	104L	37:12	0.9069	0.9037 - 0.9102	16	104L/123L/114L/					
5	108	104L	37:12	0.9069	0.9037 - 0.9102	16	104L/123L/114L/					
5	86	104L	37:17	0.9090	0.9057 - 0.9122	16	104L/123L/114L/					
5	97	104L	37:17	0.9090	0.9057 - 0.9122	16	104L/123L/114L/					
5	125	104L	37:21	0.9106	0.9074 - 0.9139	16	104L/123L/114L/					
5	87	104L	37:25	0.9122	0.9102 - 0.9143	10	104L/123L/114L/					

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EDMLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

5	108/119/8	104L	37:19	0.9098	0.9065 - 0.9130	16	104L/123L/114L/	149	475	15	48	24
5	117	104L	37:57	0.9252	0.9228 - 0.9277	12	104L/123L/114L/					
5	116	104L	38:02	0.9273	0.9248 - 0.9297	12	104L/123L/114L/					
5	85	104L	38:05	0.9285	0.9265 - 0.9305	10	104L/123L/114L/					
5	117/116/8	104L	38:00	0.9265	0.9240 - 0.9289	12	104L/123L/114L/	104	332	10	33	17
5	110	104L	38:16	0.9330	0.9309 - 0.9350	10	104L/123L/114L/					
5	115	104L	38:18	0.9338	0.9317 - 0.9358	10	104L/123L/114L/					
5	110/115	104L	38:17	0.9334	0.9313 - 0.9354	10	104L/123L/114L/	243	773	24	77	39
5	82	104L	38:40	0.9427	0.9415 - 0.9439	6	104L/123L/114L/	133	423	13	42	21
5	111	104L	38:52	0.9476	0.9464 - 0.9488	6	104L/123L/114L/	243	773	24	77	39
5	120	104L	39:21	0.9594	0.9581 - 0.9606	6	104L/123L/114L/	147	467	15	47	23
5	107	104L	40:39	0.9911	0.9890 - 0.9931	10	104L/123L/114L/					
5	124	104L	40:40	0.9915	0.9894 - 0.9935	10	104L/123L/114L/					
5	107/124	104L	40:39	0.9911	0.9890 - 0.9931	10	104L/123L/114L/	271	863	27	86	43
5	109	104L	40:54	0.9972	0.9959 - 0.9984	6	104L/123L/114L/	103	328	10	33	16
5	123	123L	41:02	1.0004	0.9992 - 1.0016	6	123L	150	476	15	48	24
5	106	123L	41:10	1.0037	1.0024 - 1.0049	6	104L/123L/114L/	143	454	14	45	23
5	118	118L	41:22	1.0004	0.9992 - 1.0016	6	118L	193	614	19	61	31
5	122	118L	41:49	1.0113	1.0101 - 1.0125	6	104L/123L/114L/	117	372	12	37	19
5	114	114L	41:58	1.0004	0.9992 - 1.0016	6	114L	120	382	12	38	19
5	105	105L	42:43	0.9996	0.9984 - 1.0008	6	105L	109	348	11	35	17
5	127	105L	44:09	1.0332	1.0320 - 1.0343	6	104L/123L/114L/	278	884	28	88	44
5	126	126L	45:58	1.0004	0.9993 - 1.0015	6	126L	136	433	14	43	22
LABELLED COMPOUNDS												
IUPAC #												
5	104L	101L	29:46	0.8257	0.8211 - 0.8303	20	101L					
5	123L	101L	41:01	1.1378	1.1331 - 1.1424	20	101L					
5	118L	101L	41:21	1.1470	1.1424 - 1.1516	20	101L					
5	114L	101L	41:57	1.1637	1.1590 - 1.1683	20	101L					
5	105L	101L	42:44	1.1854	1.1808 - 1.1900	20	101L					
5	126L	101L	45:57	1.2746	1.2700 - 1.2792	20	101L					
QUAN												

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EMDLs), and Estimated Minimum Levels (EMLs)
for the 209 PCB congeners on SPB-Octyl.

Compounds using 138L (13C12-2,2',3,4,4',5'-HxCB) as Internal Standard												
NATIVE ANALYTES												
IUPAC #	RT REFERENCE (6)	RT (8)	RRT	RRT QC LIMITS (1)	Window (7)	QUAN						
Hexachlorobiphenyls												
6	155	155L	35:44	1.0000	0.9977 - 1.0023	10	155L	339	1079	34	108	54
6	152	155L	36:07	1.0107	1.0093 - 1.0121	6	155L/156L/157L/	238	757	24	76	38
6	150	155L	36:15	1.0145	1.0131 - 1.0159	6	155L/156L/157L/	328	1044	33	104	52
6	136	155L	36:44	1.0280	1.0266 - 1.0294	6	155L/156L/157L/	91	290	9	29	14
6	145	155L	37:00	1.0354	1.0340 - 1.0368	6	155L/156L/157L/	317	1009	32	101	50
6	148	155L	34:26	1.0756	1.0742 - 1.0770	6	155L/156L/157L/	324	1030	32	103	52
6	151	155L	39:10	1.0961	1.0938 - 1.0984	10	155L/156L/157L/					
6	135	155L	39:17	1.0993	1.0970 - 1.1017	10	155L/156L/157L/					
6	154	155L	39:21	1.1012	1.0989 - 1.1035	10	155L/156L/157L/					
6	151/135/1	155L	39:15	1.0984	1.0961 - 1.1007	10	155L/156L/157L/	112	358	11	36	18
6	144	155L	39:47	1.1133	1.1119 - 1.1147	6	155L/156L/157L/	167	531	17	53	27
6	147	155L	40:09	1.1236	1.1213 - 1.1259	10	155L/156L/157L/					
6	149	155L	40:12	1.1250	1.1227 - 1.1273	10	155L/156L/157L/					
6	147/149	155L	40:10	1.1241	1.1217 - 1.1264	10	155L/156L/157L/	179	568	18	57	28
6	134	155L	40:27	1.1320	1.1297 - 1.1343	10	155L/156L/157L/					
6	143	155L	40:30	1.1334	1.1311 - 1.1357	10	155L/156L/157L/					
6	134/143	155L	40:29	1.1329	1.1306 - 1.1353	10	155L/156L/157L/	134	426	13	43	21
6	139	155L	40:47	1.1413	1.1390 - 1.1437	10	155L/156L/157L/					
6	140	155L	40:48	1.1418	1.1395 - 1.1441	10	155L/156L/157L/					
6	139/140	155L	40:47	1.1413	1.1390 - 1.1437	10	155L/156L/157L/	196	622	20	62	31
6	131	155L	41:03	1.1488	1.1474 - 1.1502	6	155L/156L/157L/	121	384	12	38	19
6	142	155L	41:13	1.1535	1.1521 - 1.1549	6	155L/156L/157L/	311	988	31	99	49
6	132	155L	41:36	1.1642	1.1618 - 1.1665	10	155L/156L/157L/	125	396	12	40	20
6	133	155L	41:57	1.1740	1.1726 - 1.1754	6	155L/156L/157L/	169	539	17	54	27
6	165	167L	42:23	0.8864	0.8853 - 0.8874	6	155L/156L/157L/	361	1149	36	115	57
6	146	167L	42:38	0.8916	0.8906 - 0.8926	6	155L/156L/157L/	182	579	18	58	29
6	161	167L	42:47	0.8947	0.8937 - 0.8958	6	155L/156L/157L/	352	1121	35	112	56

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EMDLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

6	153	167L	43:17	0.9052	0.9035 - 0.9069	10	155L/156L/157L/						
6	168	167L	43:21	0.9066	0.9048 - 0.9083	10	155L/156L/157L/						
6	153/168	167L	43:19	0.9059	0.9041 - 0.9076	10	155L/156L/157L/	130	413	13	41		21
6	141	167L	43:34	0.9111	0.9101 - 0.9122	6	155L/156L/157L/	93	295	9	30		15
6	130	167L	44:01	0.9205	0.9195 - 0.9216	6	155L/156L/157L/	136	433	14	43		22
6	137	167L	44:14	0.9251	0.9240 - 0.9261	6	155L/156L/157L/	300	954	30	95		48
6	164	167L	44:22	0.9278	0.9268 - 0.9289	6	155L/156L/157L/	136	434	14	43		22
6	138	167L	44:42	0.9348	0.9324 - 0.9373	14	155L/156L/157L/						
6	163	167L	44:42	0.9348	0.9324 - 0.9373	14	155L/156L/157L/						
6	129	167L	44:47	0.9366	0.9341 - 0.9390	14	155L/156L/157L/						
6	160	167L	44:53	0.9387	0.9369 - 0.9404	10	155L/156L/157L/						
6	138/163/1	167L	44:47	0.9366	0.9341 - 0.9390	14	155L/156L/157L/	211	671	21	67		34
6	158	167L	45:05	0.9428	0.9418 - 0.9439	6	155L/156L/157L/	96	307	10	31		15
6	166	167L	45:59	0.9617	0.9599 - 0.9634	10	155L/156L/157L/						
6	128	167L	46:46	0.9651	0.9634 - 0.9669	10	155L/156L/157L/						
6	128/166	167L	46:04	0.9634	0.9617 - 0.9651	10	155L/156L/157L/	124	393	12	39		20
6	159	167L	46:59	0.9826	0.9815 - 0.9836	6	155L/156L/157L/	348	1107	35	111		55
6	162	167L	47:18	0.9892	0.9881 - 0.9902	6	155L/156L/157L/	355	1128	35	113		56
6	167	167L	47:49	1.0000	0.9990 - 1.0010	6	155L/156L/157L/	115	364	11	36		18
6	156	156L/157L	49:05	0.9993	0.9983 - 1.0003	6	156L/157L						
6	157	156L/157L	49:09	1.0007	0.9990 - 1.0024	10	156L/157L						
6	156/157	156L/157L	45:07	1.0000	0.9990 - 1.0010	6	156L/157L	132	420	13	42		21
6	169	169L	52:31	0.9949	0.9940 - 0.9959	6	169L	161	513	16	51		26
LABELLED COMPOUNDS													
IUPAC #							IUPAC # (2)						
6	155L	138L	35:44	0.7997	0.7960 - 0.8034	20	138L						
6	167L	138L	47:49	1.0701	1.0664 - 1.0739	20	138L						
6	156L	138L	49:05	1.0985	1.0974 - 1.0996	6	138L						
6	157L	138L	49:08	1.0996	1.0959 - 1.1033	20	138L						
6	156L/157L	138L	49:07	1.0992	1.0981 - 1.1003	6	138L						
6	169L	138L	52:30	1.1749	1.1738 - 1.1761	6	138L						

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EMDLs), and Estimated Minimum Levels (EMLs)
for the 209 PCB congeners on SPB-Octyl.

Compounds using 194L(13C12-22'33'44'55'-OcCB) as Internal Standard												
NATIVE ANALYTES												
IUPAC #	RT REFERENCE (6)	RT (8)	RRT	RRT QC LIMITS (1)	Window (7)	QUAN						
Heptachlorobiphenyls												
7	188	188L	41:51	1.0000	0.9988 - 1.0012	6	188L	235	746	23	75	37
7	179	188L	42:19	1.0112	1.0100 - 1.0123	6	188L/189L	229	727	23	73	36
7	184	188L	42:45	1.0215	1.0203 - 1.0227	6	188L/189L	403	1281	40	128	64
7	176	188L	43:15	1.0335	1.0323 - 1.0346	6	188L/189L	385	1225	39	123	61
7	186	188L	43:45	1.0454	1.0442 - 1.0466	6	188L/189L	407	1295	41	129	65
7	178	188L	45:06	1.0777	1.0765 - 1.0789	6	188L/189L	221	703	22	70	35
7	175	188L	45:46	1.0936	1.0924 - 1.0948	6	188L/189L	383	1218	38	122	61
7	187	188L	46:02	1.1000	1.0988 - 1.1012	6	188L/189L	191	609	19	61	30
7	182	180L	46:14	0.9164	0.9154 - 0.9174	6	188L/189L	398	1267	40	127	63
7	183	180L	46:42	0.9257	0.9247 - 0.9267	6	188L/189L					
7	185	180L	46:53	0.9293	0.9283 - 0.9303	6	188L/189L					
7	183/185	180L	46:47	0.9273	0.9263 - 0.9283	6	188L/189L	401	1274	40	127	64
7	174	180L	47:02	0.9323	0.9313 - 0.9333	6	188L/189L	186	591	19	59	30
7	177	180L	47:30	0.9415	0.9405 - 0.9425	6	188L/189L	141	448	14	45	22
7	181	180L	47:52	0.9488	0.9478 - 0.9498	6	188L/189L	396	1260	40	126	63
7	171	180L	48:10	0.9547	0.9531 - 0.9564	10	188L/189L					
7	173	180L	48:11	0.9551	0.9541 - 0.9561	6	188L/189L					
7	171/173	180L	48:10	0.9547	0.9531 - 0.9564	10	188L/189L	374	1190	37	119	60
7	172	180L	49:47	0.9868	0.9858 - 0.9878	6	188L/189L	377	1197	38	120	60
7	192	180L	50:06	0.9931	0.9921 - 0.9941	6	188L/189L	420	1337	42	134	67
7	193	180L	50:26	0.9997	0.9987 - 1.0007	6	188L/189L					
7	180	180L	50:27	1.0000	0.9990 - 1.0010	6	188L/189L					
7	180/193	180L	50:26	0.9997	0.9987 - 1.0007	6	188L/189L	136	432	14	43	22
7	191	180L	50:51	1.0079	1.0069 - 1.0089	6	188L/189L	418	1330	42	133	66
7	170	180L	51:54	1.0287	1.0278 - 1.0297	6	188L/189L	162	516	16	52	26
7	190	180L	52:26	1.0393	1.0383 - 1.0403	6	188L/189L	234	743	23	74	37

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EDMLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

7	189	189L	55:07	1.0003	0.9994 - 1.0012	6	189L	177	564	18	56	28
Octachlorobiphenyls												
8	202	202L	47:32	1.0004	0.9986 - 1.0021	10	202L	442	1406	44	141	70
8	201	202L	48:31	1.0210	1.0193 - 1.0228	10	202L/205L	440	1399	44	140	70
8	204	202L	49:11	1.0351	1.0340 - 1.0361	6	202L/205L	447	1420	45	142	71
8	197	202L	49:27	1.0407	1.0396 - 1.0417	6	202L/205L					
8	200	202L	49:40	1.0452	1.0442 - 1.0463	6	202L/205L					
8	197/200	202L	49:33	1.0428	1.0417 - 1.0438	6	202L/205L	245	780	25	78	39
8	198	202L	52:30	1.1049	1.1031 - 1.1066	10	202L/205L					
8	199	202L	52:32	1.1056	1.1045 - 1.1066	6	202L/205L					
8	198/199	202L	52:31	1.1052	1.1035 - 1.1070	10	202L/205L	203	647	20	65	32
8	196	205L	53:13	0.9207	0.9198 - 0.9216	6	202L/205L	429	1364	43	136	68
8	203	205L	53:26	0.9245	0.9236 - 0.9253	6	202L/205L	444	1413	44	141	71
8	195	205L	54:55	0.9501	0.9493 - 0.9510	6	202L/205L	427	1357	43	136	68
8	194	205L	57:19	0.9916	0.9908 - 0.9925	6	202L/205L	170	539	17	54	27
8	205	205L	57:49	1.0003	0.9994 - 1.0012	6	205L	449	1427	45	143	71
Nonachlorobiphenyls												
9	208	208L	54:33	1.0003	0.9994 - 1.0012	6	208L	455	1448	46	145	72
9	207	208L	55:32	1.0183	1.0174 - 1.0193	6	208L/206L	453	1441	45	144	72
9	206	206L	59:37	1.0003	0.9994 - 1.0011	6	206L	451	1434	45	143	72
Decachlorobiphenyl												
10	209	209L	61:15	1.0003	0.9995 - 1.0011	6	209L	153	486	15	49	24
LABELLED COMPOUNDS												
	IUPAC #	RT REFERENCE (6)					QUAN					
7	188L	194L	41:51	0.7304	0.7275 - 0.7333	20	194L					
7	180L	194L	50:27	0.8805	0.8775 - 0.8834	20	194L					
7	170L	194L	51:53	0.9055	0.9026 - 0.9084	20	194L					
7	189L	194L	55:06	0.9616	0.9587 - 0.9645	20	194L					
8	202L	194L	47:31	0.8293	0.8264 - 0.8322	20	194L					
8	205L	194L	57:48	1.0087	1.0044 - 1.0131	30	194L					

Table 18. (continued) Retention time (RT) references, Quantitation References, Relative Retention Times (RRTs), Estimated Detection Limits (EMDLs), and Estimated Minimum Levels (EMLs) for the 209 PCB congeners on SPB-Octyl.

9	208L	194L	54:32	0.9517	0.9488 - 0.9546	20	194L	
9	206L	194L	59:36	1.0401	1.0358 - 1.0445	30	194L	
10	209L	194L	61:14	1.0686	1.0643 - 1.0730	30	194L	
LABELED CLEAN-UP								
3	28L	52L	26:44	0.9266	0.9209 - 0.9324	20	52L	0
5	111L	101L	38:51	1.0777	1.0730 - 1.0823	20	101L	
7	178L	138L	45:05	1.0090	1.0052 - 1.0127	20	138L	1
LABELLED INTERNAL AND RETENTION TIME STANDARDS								
2	9L	138L	18:54	0.4648	0.4596 - 0.4699	25		
4	52L	138L	28:51	0.7094	0.7043 - 0.7145	25		
5	101L	138L	36:03	0.8865	0.8814 - 0.8916	25		
6	138L	138L	44:41	1.0988	1.0783 - 1.1193	100		
8	194L	138L	57:18	1.4090	1.4039 - 1.4141	25		

(1) QC limits for Relative Retention Times (RRT) are based on +/- 0.5 of the targetting window width used to locate peaks.

(2) Suffix "L" indicates labelled compound.

(3) Clean-up standard

(4) Primary retention time standard. Quantitated by the external standard method

(5) Secondary retention time standards. Quantitated by the external standard method.

(6) Retention time reference compounds used to locate target compound.

(7) Labeled compound (or group of isomers) used as quantitation reference(s)

(8) Width in seconds of retention time window for targeted congener or domain of two or more congeners

(9) Typical retention times in listed (min:sec) for a 30 m SPB Octyl column. These are determined from the daily calibration standard containing all 209 congeners

(10) A box indicates a "domain" of congeners that co-elute or may not be adequately resolved on a 30m Octyl. Congeners included in the domain are indicated as the last item in each

(11) This Table is listed in Method 1668, Rev as Table 2 in has been

Table 19. QC acceptance criteria for chlorinated biphenyls in VER, IPR, OPR and samples

CB Congener	IUPAC ¹	Test conc. (ng/mL)	VER (%)	IPR		OPR (%)	Labeled compound Recovery in samples (%)
Native Toxic/LOC				RSD	X (%)		
2-CB	1	50	70-130	40	60-140	50-150	
4-CB	3	50	70-130	40	60-140	50-150	
2,2'-DiCB	4	50	70-130	40	60-140	50-150	
4,4'-DiCB	15	50	70-130	40	60-140	50-150	
2,2'6'-TrCB	19	50	70-130	40	60-140	50-150	
2,4,4'-TrCB	37	50	70-130	40	60-140	50-150	
2,2',6,6'-TeCB	54	50	70-130	40	60-140	50-150	
3,3',4,4'-TeCB	77	50	70-130	40	60-140	50-150	
3,4,4',5'-TeCB	81	50	70-130	40	60-140	50-150	
2,2',4,6,6'-PeCB	104	50	70-130	40	60-140	50-150	
2,3,3',4,4'-PeCB	105	50	70-130	40	60-140	50-150	
2,3,4,4',5-PeCB	114	50	70-130	40	60-140	50-150	
2,3',4,4',5-PeCB	118	50	70-130	40	60-140	50-150	
2',3,4,4',5-PeCB	123	50	70-130	40	60-140	50-150	
3,3',4,4',5-PeCB	126	50	70-130	40	60-140	50-150	
2,2,4,4,6,6'-HxCB	155	50	70-130	40	60-140	50-150	
2,3,3',4,4',5-HxCB	156	50	70-130	40	60-140	50-150	
2,3,3',4,4',5'-HxCB	157	50	70-130	40	60-140	50-150	
3,3',4,4',5,5'-HxCB	169	50	70-130	40	60-140	50-150	
2,2',3,4',5,6,6'-HpCB	188	50	70-130	40	60-140	50-150	
2,3,3',4,4',5,5'-HpCB	189	50	70-130	40	60-140	50-150	
2,2',3,3',5,5,6,6''-OcCB	202	50	70-130	40	60-140	50-150	
2,3,3',4,4',5,5,6-OcCB	205	50	70-130	40	60-140	50-150	
2,2',3,3',4,4',5,5,6'-NoCB	206	50	70-130	40	60-140	50-150	
2,2',3,3',4',5,5,6,6'-NCB	208	50	70-130	40	60-140	50-150	
DeCB	209	50	70-130	40	60-140	50-150	
<hr/>							
Labeled toxic/LOC							
13C12-2-CB	1L	100	50-150	50	35-135	30-140	25-150
13C12-4-CB	3L	100	50-150	50	35-135	30-140	25-150
13C12-2,2''-DiCB	4L	100	50-150	50	35-135	30-140	25-150

Table 19. (continued) QC acceptance criteria for chlorinated biphenyl congeners in VER,IPR, OPR and samples

CB Congener	IUPAC¹	Test conc. (ng/mL)	VER (%)	IPR		OPR (%)	Labeled compound Recovery in samples (%)
Native Toxic/LOC				RSD	X (%)		
13C12-4,4'-DiCB	15L	100	50-150	50	35-135	30-140	25-150
13C12-2,2'6'-TrCB	19L	100	50-150	50	35-135	30-140	25-150
13C12-2,4,4'-TrCB	37L	100	50-150	50	35-135	30-140	25-150
13C12-2,2',6,6'-TeCB	54L	100	50-150	50	35-135	30-140	25-150
13C12-3,3',4,4'-TeCB	77L	100	50-150	50	35-135	30-140	25-150
13C12-3,4,4',5'-TeCB	81L	100	50-150	50	35-135	30-140	25-150
13C12-2,2',4,6,6'-PeCB	104L	100	50-150	50	35-135	30-140	25-150
13C12-2,3,3',4,4'-PeCB	105L	100	50-150	50	35-135	30-140	25-150
13C12-2,3,4,4',5-PeCB	114L	100	50-150	50	35-135	30-140	25-150
13C12-2,3',4,4',5-PeCB	118L	100	50-150	50	35-135	30-140	25-150
13C12-2',3,4,4',5-PeCB	123L	100	50-150	50	35-135	30-140	25-150
13C12-3,3',4,4',5-PeCB	126L	100	50-150	50	35-135	30-140	25-150
13C12-2,2,4,4,6,6'-HxCB	155L	100	50-150	50	35-135	30-140	25-150
13C12-2,3,3',4,4',5-HxCB	156L	100	50-150	50	35-135	30-140	25-150
13C12-2,3,3',4,4',5'-HxCB	157L	100	50-150	50	35-135	30-140	25-150
13C12-3,3',4,4',5,5'-HxCB	169L	100	50-150	50	35-135	30-140	25-150
13C12-2,2',3,4',5,6,6'-HpCB	188L	100	50-150	50	35-135	30-140	25-150
13C12-2,3,3',4,4',5,5'-HpCB	189L	100	50-150	50	35-135	30-140	25-150
13C12-2,2',3,3',5,5,6,6'-OcCB	202L	100	50-150	50	35-135	30-140	25-150
13C12-2,3,3',4,4',5,5,6-OcCB	205L	100	50-150	50	35-135	30-140	25-150
13C12-2,2',3,3',4,4',5,5,6'-NoCB	206L	100	50-150	50	35-135	30-140	25-150
13C12-2,2',3,3',4',5,5,6,6'-NoCB	208L	100	50-150	50	35-135	30-140	25-150
13C12-DeCB	209L	100	50-150	50	35-135	30-140	25-150
Labeled cleanup standard							
13C12-2,4,4'-TCB	28L	100	6--130	45	45-120	40-125	30-135
13C12-2,3,3',5,5'-PeCB	111L	100	6--130	45	45-120	40-125	30-135
13C12-2,2',3,3',5,5',6,-HpCB	178L	100	6--130	45	45-120	40-125	30-135

1. QC acceptance criteria for IPR,OPR and samples based on a 20 μ L final extract volume.
2. Suffix "L" indicated a labeled compound
3. See table 18
4. PCBs 156 and 157 are tested as the sum of two concentrations

Table A1. Aroclor 1221 : Congener concentrations (wt%) and comparison to published values

(Refer to footnotes for Table 15 for explanation of headings)

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn. wt %	SDL wt %	RA wt %	RA? wt %	S.P.D. MS wt %	G.Frame wt %	G.Fram wt %
1	Octyl		32.209	0.00	3.10	y		31.09	23.41
2	Octyl		3.066	0.00	3.09	y		2.85	
3	Octyl		17.449	0.00	3.09	y		15.58	14.57
4	Octyl		5.806	0.29	1.43	y		5.85	5.17
5	Octyl		0.845	0.23	1.36	y		0.64	0.80
6	Octyl		3.4	0.22	1.43	y		2.67	3.15
7	Octyl		1.556	0.20	1.37	y		1.13	1.77
8	Octyl		10.885	0.21	1.49	y		9.52	10.10
9	Octyl		1.761	0.22	1.33	y		1.17	1.59
10	Octyl		0.727	0.23	0.96	n		0.41	0.56
11	Octyl		0.108	0.24	1.67	y		0.09	
12	Octyl	12+13	see 13	0.25	1.43	y		0.44	0.76
13	Octyl	12+13	1.657	0.25	1.43	y		0.98	1.16
14	Octyl		0.013	0.24	0.41	n		0.02	
15	Octyl		3.651	0.24	1.42	y		3.20	4.54
16	Octyl		0.242	0.02	1.02	y		0.26	0.41
17	Octyl		0.29	0.02	0.92	y		0.33	0.43
18	DB-1		0.44	0.03	1.00	y		0.64	0.89
19	Octyl		0.067	0.02	1.06	y		0.07	0.15
20	Octyl	28+20	see 28	0.02	1.02	y		0.05	0.09
21	Octyl	21+33	see 33	0.02	1.00	y			
22	Octyl		0.14	0.02	0.92	y		0.20	0.30
23	Octyl		0	0.02	*	n		0.00	0.03
24	Octyl		0.007	0.01	0.27	n		0.02	0.05
25	Octyl		0.068	0.01	1.07	y		0.08	0.16
26	DB-1		0.09	0.02	1.25	n		0.10	0.19
27	Octyl		0.042	0.01	0.80	n		0.05	0.25
28	Octyl	28+20	0.397	0.02	1.02	y		0.46	0.76
29	DB-1		0	0.02	*	n		0.02	0.03
30	DB-1		0.003	0.02	0.80	n			
31	Octyl		0.317	0.01	1.01	y		0.46	0.65
32	Octyl		0.112	0.02	1.18	y		0.13	0.22
33	Octyl	21+33	0.274	0.02	1.00	y		0.39	0.62
34	Octyl		0	0.02	*	n			
35	Octyl		0.009	0.02	0.37	n		0.02	

Table A1. (continued) Aroclor 1221 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D. MS	G.Frame	G.Fram ECD
36	Octyl		0	0.02	*	n			
37	Octyl		0.076	0.02	0.74	n	0.15	0.22	
38	Octyl		0.003	0.02	2.24	n			
39	Octyl		0	0.02	*	n			
40	DB-1		0	0.01	*	n	0.04	0.07	
41	Octyl		0	0.01	*	n	0.23	0.06	
42	Octyl		0	0.01	*	n	0.08	0.10	
43	Octyl		0	0.01	*	n		0.30	
44	DB-1		0.067	0.01	0.61	n	0.16	0.27	
45	DB-1		0	0.01	*	n	0.05	0.10	
46	Octyl		0	0.01	*	n	0.02		
47	DB-1		0	0.01	*	n	0.05	0.08	
48	Octyl		0.017	0.01	0.75	y	0.07	0.10	
49	Octyl	69+49	0.035	0.01	1.36	n	0.15	0.20	
50	DB-1		0	0.01	*	n	0.02	0.12	
51	DB-1		0	0.01	*	n	0.01	0.07	
52	Octyl		0.071	0.01	0.43	n	0.18	0.30	
53	DB-1		0	0.01	*	n	0.04	0.03	
54	Octyl		0	0.01	*	n			
55	Octyl		0	0.02	*	n	0.01	0.02	
56	Octyl		0	0.02	*	n	0.14	0.14	
57	Octyl		0	0.02	*	n			
58	Octyl		0	0.02	*	n			
59	Octyl	59+62+75	0	0.01	*	n	0.02	0.04	
60	Octyl		0	0.02	*	n	0.15	0.12	
61	DB-1	74+61	see 74	0.02	*	n			
62	DB-1	65+62	0	0.02	*	n			
63	Octyl		0	0.02	*	n	0.01	0.02	
64	Octyl		0.025	0.01	0.55	n	0.08	0.14	
65	DB-1	65+62	see 62	0.02	*	n		0.11	
66	Octyl		0.027	0.02	0.63	n	0.16	0.26	
67	Octyl		0	0.02	*	n	0.01	0.09	
68	Octyl		0	0.02	*	n			
69	Octyl	69+49	see 49	0.01	1.36	n			
70	DB-1		0	0.01	*	n	0.15	0.27	
71	Octyl	40+71	see 40	0.01	0.91	n	0.04	0.10	
72	Octyl		0	0.02	*	n			
73	Octyl		0	0.01	*	n			
74	DB-1	74+61	0	0.02	*	n	0.09	0.15	
75	Octyl	59+62+75	see 59	0.01	*	n			

Table A1. (continued) Aroclor 1221 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D. MS	G.Frame	G.Fram ECD
76	Octyl	61+70+74+76	see 70	0.02	0.52	n			
77	Octyl		0	0.02	*	n		0.02	
78	Octyl		0	0.02	*	n			
79	Octyl		0	0.02	*	n			
80	Octyl		0	0.02	*	n			
81	Octyl		0	0.02	*	n			0.07
82	Octyl		0	0.01	*	n	0.02	0.03	
83	DB-1	83+112	0	0.06	*	n			
84	Octyl		0	0.01	*	n	0.04	0.07	
85	Octyl	117+116+85	0	0.01	*	n	0.03	0.04	
86	DB-1		0	0.08	*	n			
87	Octyl	108+119+86+97+125 +87	0	0.01	*	n	0.04	0.07	
88	DB-1		0	0.07	*	n			
89	Octyl		0	0.01	*	n			
90	Octyl	113+90+101	see 101	0.01	1.73	y			
91	DB-1		0	0.07	*	n	0.01		
92	Octyl		0	0.01	*	n	0.01	0.83	
93	Octyl	100+93	0	0.01	*	n			
94	Octyl		0	0.01	*	n			
95	Octyl		0.099	0.01	1.51	y	0.05	0.10	
96	Octyl		0	0.01	*	n			
97	DB-1		0	0.07	*	n	0.03	0.06	
98	Octyl	102+98	see 102	0.01	*	n			
99	Octyl	83+99	0	0.01	*	n	0.03	0.08	
100	DB-1		0	0.07	*	n			
101	Octyl	113+90+101	0.099	0.01	1.73	y	0.05	0.12	
102	Octyl	102+98	0	0.01	*	n	0.00		
103	Octyl		0	0.01	*	n			
104	Octyl		0	0.01	*	n			
105	Octyl		0	0.01	*	n	0.05	0.06	
106	Octyl		0	0.01	*	n			
107	Octyl	107+124	see 124	0.01	*	n			
108	DB-1		0	0.06	*	n			
109	Octyl		0	0.01	*	n	0.00		
110	Octyl	110+115	0.042	0.01	2.26	n	0.06	0.13	
111	Octyl		0	0.01	*	n			
112	Octyl		0	0.01	*	n			
113	Octyl	113+90+101	see 101	0.01	1.73	y			
114	Octyl		0	0.01	*	n	0.00		

Table A1. (continued) Aroclor 1221 : Congener concentrations (wt%) and comparison to published values

Congener	Reporting	Co-eluting	Congener	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
IUPAC#	column	isomers	Concn.				MS		ECD
115	Octyl	110+115	see 110	0.01	2.26	n			
116	Octyl	117+116+85	see 85	0.01	*	n			
117	Octyl	117+116+85	see 85	0.01	*	n			
118	Octyl		0	0.01	*	n	0.05	0.11	
119	DB-1		0	0.05	*	n			
120	Octyl		0	0.01	*	n		0.03	
121	Octyl		0	0.01	*	n			
122	Octyl		0	0.01	*	n			
123	Octyl		0	0.01	*	n			
124	Octyl	107+124	0	0.01	*	n	0.00		
125	Octyl	108+119+86+97+125 +87	see 97	0.01	*	n			
126	Octyl		0	0.02	*	n			
127	Octyl		0	0.01	*	n			
128	DB-1		0	0.01	*	n	0.01		
129	DB-1		0	0.01	*	n		0.20	
130	Octyl		0	0.01	*	n			
131	Octyl		0	0.01	*	n			
132	Octyl		0.039	0.01	1.27	y	0.01		
133	Octyl		0	0.00	*	n			
134	Octyl	134+143	0	0.01	*	n		0.11	
135	Octyl	151+135	0.097	0.02	0.74	n			
136	Octyl		0.026	0.01	1.69	n			
137	Octyl		0	0.01	*	n			
138	DB-1	138+163+164	0.078	0.01	1.55	n	0.02	0.03	
139	Octyl	139+140	0	0.00	*	n			
140	DB-1		0	0.01	*	n			
141	Octyl		0	0.00	*	n			
142	Octyl		0	0.01	*	n			
143	Octyl	134+143	see 134	0.01	*	n			
144	Octyl		0	0.01	*	n		0.02	
145	Octyl		0	0.01	*	n			
146	Octyl		0	0.00	*	n		0.04	
147	DB-1		0	0.01	*	n			
148	Octyl		0	0.01	*	n			
149	DB-1	139+149	0.145	0.01	1.13	y	0.01		
150	Octyl		0	0.01	*	n			
151	DB-1		0	0.01	*	n			
152	Octyl		0	0.01	*	n			
153	DB-1		0.083	0.01	0.94	n	0.01	0.06	

Table A1. (continued) Aroclor 1221 : Congener concentrations (wt%) and comparison to published values

Congener	Reporting	Co-eluting	Congener	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
IUPAC#	column	isomers	Concn.				MS		ECD
154	Octyl		0	0.01	*	n			
155	Octyl		0	0.01	*	n			
156	DB-1		0	0.01	*	n			
157	DB-1		0	0.01	*	n			
158	Octyl		0	0.00	*	n			
159	Octyl		0	0.00	*	n			
160	DB-1	158+160	0	0.01	*	n			
161	Octyl		0	0.00	*	n			
162	Octyl		0	0.00	*	n			
163	Octyl	138+163+129+160	see 138	0.01	2.43	n			
164	Octyl		0	0.00	*	n			0.01
165	Octyl		0	0.00	*	n			
166	DB-1		0	0.01	*	n			
167	Octyl		0	0.00	*	n			
168	DB-1		0	0.01	*	n			
169	Octyl		0	0.01	*	n			
170	Octyl		0	0.01	*	n			0.09
171	DB-1		0	0.02	*	n			0.02
172	Octyl		0	0.01	*	n			
173	DB-1		0	0.02	*	n			
174	Octyl		0.017	0.01	1.23	n			
175	Octyl		0	0.01	*	n			
176	Octyl		0	0.01	*	n			
177	Octyl		0	0.01	*	n			
178	Octyl		0	0.01	*	n			
179	Octyl		0.018	0.01	0.57	n			
180	DB-1		0.042	0.02	0.78	n			0.06
181	Octyl		0	0.01	*	n			
182	Octyl		0	0.01	*	n			
183	Octyl		0.014	0.01	0.78	n			
184	Octyl		0	0.01	*	n			
185	Octyl		0	0.01	*	n			
186	Octyl		0	0.01	*	n			
187	Octyl		0.016	0.01	0.25	n			0.08
188	Octyl		0	0.01	*	n			
189	Octyl		0	0.02	*	n			
190	Octyl		0	0.01	*	n			
191	Octyl		0	0.01	*	n			
192	Octyl		0	0.01	*	n			
193	DB-1		0	0.02	*	n			
194	Octyl		0	0.02	*	n			

Table A1. (continued) Aroclor 1221 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D. MS	G.Frame	G.Fram ECD
195	Octyl		0	0.02	*	n			
196	Octyl		0	0.02	*	n			
197	Octyl		0	0.01	*	n			
198	DB-1		0	0.02	*	n			
199	DB-1		0	0.02	*	n			
200	Octyl		0	0.01	*	n			
201	Octyl		0	0.01	*	n			0.09
202	Octyl		0	0.01	*	n			
203	Octyl		0	0.02	*	n			
204	Octyl		0	0.01	*	n			
205	Octyl		0	0.02	*	n			
206	Octyl		0	0.05	*	n		0.05	0.08
207	Octyl		0	0.03	*	n			0.01
208	Octyl		0	0.03	*	n		0.02	0.04
209	Octyl		0	0.02	*	n			

Homologue Totals

Cl-1	52.72 wt %
Cl-2	30.41 wt %
Cl-3	2.57 wt %
Cl-4	0.25 wt %
Cl-5	0.24 wt %
Cl-6	0.47 wt %
Cl-7	0.11 wt %
Cl-8	0.00 wt %
Cl-9	0.00 wt %
Cl-10	0.00 wt %

86.77 wt %

Table A2. Aroclor 1232: Congener concentrations (wt%) and comparison to published values

(Refer to footnotes for table 15 for explanation of headings)

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL wt %	RA wt %	RA? wt %	S.P.D. MS	G.Frame wt %	G.Frai wt %
1	Octyl		16.467	0.00	3.07	y		15.59	16.41
2	Octyl		1.65	0.00	3.10	y		0.00	1.68
3	Octyl		10.336	0.00	3.08	y		8.24	8.38
4	Octyl		3.957	0.16	1.40	y		5.16	5.16
5	Octyl		0.444	0.13	1.39	y		0.69	0.69
6	Octyl		2.208	0.12	1.45	y		2.82	2.73
7	Octyl		0.862	0.11	1.45	y		1.33	1.33
8	Octyl		8.642	0.12	1.48	y		9.12	9.12
9	Octyl		1.015	0.12	1.46	y		1.43	1.43
10	Octyl		0.391	0.12	1.06	n		0.50	0.50
11	Octyl		0.069	0.13	0.79	n		0.00	0.08
12	Octyl	12+13	see 13	0.14	1.28	n		0.00	0.42
13	Octyl	12+13	1.028	0.14	1.28	n		0.44	0.71
14	Octyl		0.007	0.13	0.52	n		0.00	0.00
15	Octyl		2.934	0.13	1.44	y		0.00	1.75
16	Octyl		1.915	0.01	0.92	y		2.91	2.21
17	Octyl		1.891	0.01	0.95	y		2.10	1.98
18	DB-1		4.249	0.01	1.02	y		4.99	4.92
19	Octyl		0.46	0.01	0.98	y		0.55	0.53
20	Octyl	28+20	see 28	0.01	1.04	y		@28	@33
21	Octyl	21+33	see 33	0.01	1.01	y		0.00	0.00
22	Octyl		1.596	0.02	1.02	y		1.93	1.79
23	Octyl		0.002	0.01	0.44	n		0.00	0.00
24	Octyl		0.067	0.01	1.07	y		0.00	0.00
25	Octyl		0.323	0.01	1.00	y		0.75	0.75
26	DB-1		0.593	0.02	1.00	y		1.08	0.98
27	Octyl		0.271	0.01	0.99	y		0.50	0.43
28	Octyl	28+20	4.156	0.01	1.04	y		4.19	3.93
29	DB-1		0.036	0.02	1.35	n		0.00	0.03
30	DB-1		0	0.01	*	n		0.00	0.00
31	Octyl		4.056	0.01	0.99	y		4.04	3.88
32	Octyl		1.077	0.02	1.09	y		1.37	1.28
33	Octyl	21+33	2.834	0.01	1.01	y		3.27	3.14
34	Octyl		0.015	0.02	0.57	n		0.00	0.01
35	Octyl		0.046	0.02	1.19	y		0.00	0.03

Table A2. (continued) Aroclor 1232: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fra ECD
							wt %	wt %	wt %
36	Octyl		0	0.01	*	n		0.00	0.00
37	Octyl		1.143	0.02	1.07	y		1.00	1.12
38	Octyl		0	0.02	*	n		0.00	0.00
39	Octyl		0	0.02	*	n		0.00	0.00
40	DB-1		0.38	0.02	0.78	y		1.32	0.44
41	Octyl		0.31	0.01	0.74	y		0.47	0.47
42	Octyl		0.607	0.01	0.78	y		0.88	0.88
43	Octyl		0.098	0.01	0.72	y		0.15	0.15
44	DB-1		2.217	0.01	0.76	y		2.31	2.06
45	DB-1		0.557	0.00	0.77	y		0.70	0.60
46	Octyl		0.189	0.01	0.75	y		0.29	0.25
47	DB-1		0.537	0.00	0.72	y		0.58	0.55
48	Octyl		0.56	0.01	0.74	y		0.84	0.77
49	Octyl	69+49	1.206	0.01	0.77	y		1.70	1.60
50	DB-1		0	0.00	*	n		0.00	0.00
51	DB-1		0.157	0.00	0.79	y		0.00	0.00
52	Octyl		1.804	0.01	0.75	y		2.06	1.90
53	DB-1		0.43	0.00	0.84	y		0.00	0.36
54	Octyl		0	0.01	*	n		0.00	0.00
55	Octyl		0.07	0.02	0.82	y		0.12	0.09
56	Octyl		0.897	0.02	0.76	y		1.16	1.16
57	Octyl		0	0.02	*	n		0.00	0.01
58	Octyl		0	0.02	*	n		0.00	0.00
59	Octyl	59+62+75	0.205	0.01	0.75	y		0.33	0.17
60	Octyl		0.579	0.02	0.76	y		0.87	0.87
61	DB-1	74+61	see 74	0.02	0.72	y		0.00	0.00
62	DB-1	65+62	0	0.01	*	n		0.00	0.00
63	Octyl		0.07	0.02	0.70	y		0.12	0.11
64	Octyl		0.918	0.01	0.73	y		1.34	1.34
65	DB-1	65+62	see 62	0.01	*	n		0.00	0.00
66	Octyl		1.54	0.02	0.76	y		2.11	1.97
67	Octyl		0.075	0.02	0.83	y		0.11	0.09
68	Octyl		0	0.02	*	n		0.00	0.00
69	Octyl	69+49	see 49	0.01	0.77	y		0.00	0.00
70	DB-1		1.777	0.01	0.77	y		2.16	1.56
71	Octyl	40+71	see 40	0.01	0.70	y		0.00	@64
72	Octyl		0	0.02	*	n		0.00	0.00
73	Octyl		0	0.01	*	n		0.00	0.00
74	DB-1	74+61	1.623	0.02	0.72	y		1.26	1.09

Table A2. (continued) Aroclor 1232: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fra ECD
							wt %	wt %	wt %
75	Octyl	59+62+75	see 59	0.01	0.75	y		0.00	0.00
76	Octyl	61+70+74+76	see 70	0.02	0.75	y		0.00	0.00
77	Octyl		0.142	0.02	0.80	y		0.25	0.20
78	Octyl		0	0.02	*	n		0.00	0.00
79	Octyl		0	0.02	*	n		0.00	0.00
80	Octyl		0	0.02	*	n		0.00	0.00
81	Octyl		0.006	0.02	0.93	n		0.00	0.00
82	Octyl		0.086	0.01	1.64	y		0.15	0.14
83	DB-1	83+112	0.037	0.04	1.32	n		0.00	0.02
84	Octyl		0.144	0.01	1.50	y		0.29	0.26
85	Octyl	117+116+85	0.09	0.01	1.66	y		0.18	0.17
86	DB-1		0	0.05	*	n		0.00	0.00
87	Octyl	108+119+86+97+125 +87	0.167	0.01	1.70	y		0.36	0.29
88	DB-1		0	0.04	*	n		0.00	0.00
89	Octyl		0.021	0.01	1.37	y		0.00	0.01
90	Octyl	113+90+101	see 101	0.01	1.55	y		0.00	0.00
91	DB-1		0.097	0.04	1.27	n		0.00	0.11
92	Octyl		0.046	0.01	2.00	n		0.14	0.14
93	Octyl	100+93	0	0.01	*	n		0.00	0.00
94	Octyl		0	0.01	*	n		0.00	0.00
95	Octyl		0.286	0.01	1.64	y		0.41	0.37
96	Octyl		0	0.01	*	n		0.00	0.00
97	DB-1		0.148	0.04	1.17	n		0.32	0.19
98	Octyl	102+98	see 102	0.01	2.73	n		0.00	0.00
99	Octyl	83+99	0.21	0.01	1.72	y		0.34	0.28
100	DB-1		0	0.04	*	n		0.00	0.00
101	Octyl	113+90+101	0.3	0.01	1.55	y		0.57	0.45
102	Octyl	102+98	0.024	0.01	2.73	n		0.00	0.00
103	Octyl		0	0.01	*	n		0.00	0.00
104	Octyl		0	0.01	*	n		0.00	0.00
105	Octyl		0.132	0.02	1.51	y		0.29	0.24
106	Octyl		0	0.02	*	n		0.00	0.00
107	Octyl	107+124	see 124	0.02	*	n		0.00	0.01
108	DB-1		0	0.03	*	n		0.00	
109	Octyl		0.014	0.02	4.84	n		0.04	0.02
110	Octyl	110+115	0.32	0.01	1.48	y		0.49	0.43
111	Octyl		0	0.01	*	n		0.00	0.00
112	Octyl		0.003	0.01	1.27	n		0.00	0.00

Table A2. (continued) Aroclor 1232: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fra ECD
							wt %	wt %	wt %
113	Octyl	113+90+101	see 101	0.01	1.55	y		0.00	0.00
114	Octyl		0	0.02	*	n		0.00	0.00
115	Octyl	110+115	see 110	0.01	1.48	y		0.00	0.01
116	Octyl	117+116+85	see 85	0.01	1.66	y		0.00	0.00
117	Octyl	117+116+85	see 85	0.01	1.66	y		0.00	0.00
118	Octyl		0.237	0.02	1.47	y		0.49	0.40
119	DB-1		0.003	0.03	2.48	n		0.00	0.00
120	Octyl		0	0.01	*	n		0.00	0.00
121	Octyl		0	0.01	*	n		0.00	0.00
122	Octyl		0	0.02	*	n		0.00	0.00
123	Octyl		0	0.02	*	n		0.00	0.00
124	Octyl	107+124	0	0.02	*	n		0.00	0.00
125	Octyl	108+119+86+97+125 +87	see 97	0.01	1.70	y		0.00	0.00
126	Octyl		0	0.02	*	n		0.00	0.00
127	Octyl		0	0.02	*	n		0.00	0.00
128	DB-1		0	0.01	*	n		0.00	0.00
129	DB-1		0	0.01	*	n		0.00	0.00
130	Octyl		0	0.01	*	n		0.00	0.00
131	Octyl		0	0.00	*	n		0.00	0.00
132	Octyl		0.024	0.00	2.58	n		0.00	0.00
133	Octyl		0	0.00	*	n		0.00	0.00
134	Octyl	134+143	0	0.01	*	n		0.00	0.00
135	Octyl	151+135	0	0.01	*	n		0.00	0.00
136	Octyl		0.015	0.00	1.60	n		0.13	0.07
137	Octyl		0	0.00	*	n		0.00	0.00
138	DB-1	138+163+164	0.08	0.01	1.39	y		0.11	0.08
139	Octyl	139+140	0	0.00	*	n		0.00	0.00
140	DB-1		0	0.01	*	n		0.00	0.00
141	Octyl		0.02	0.00	1.86	n		0.00	0.00
142	Octyl		0	0.00	*	n		0.00	0.00
143	Octyl	134+143	see 134	0.01	*	n		0.00	0.00
144	Octyl		0	0.00	*	n		0.00	0.00
145	Octyl		0	0.00	*	n		0.00	0.00
146	Octyl		0.005	0.00	7.97	n		0.00	0.00
147	DB-1		0	0.01	*	n		0.00	0.00
148	Octyl		0	0.00	*	n		0.00	0.00
149	DB-1	139+149	0.088	0.01	1.32	y		0.06	0.06
150	Octyl		0	0.00	*	n		0.00	0.00

Table A2. (continued) Aroclor 1232: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fra ECD
							wt %	wt %	wt %
151	DB-1		0.026	0.01	3.02	n		0.00	0.00
152	Octyl		0	0.00	*	n		0.00	0.00
153	DB-1		0.059	0.01	1.63	n		0.11	0.08
154	Octyl		0	0.00	*	n		0.00	0.00
155	Octyl		0	0.00	*	n		0.00	0.00
156	DB-1		0	0.02	*	n		0.00	0.00
157	DB-1		0	0.01	*	n		0.00	0.00
158	Octyl		0.005	0.00	3.86	n		0.00	0.00
159	Octyl		0	0.00	*	n		0.00	0.00
160	DB-1	158+160	-0.005	0.01	*	n		0.00	0.00
161	Octyl		0	0.00	*	n		0.00	0.00
162	Octyl		0	0.00	*	n		0.00	0.00
163	Octyl	138+163+129+160	see 138	0.01	1.62	n		0.00	0.00
164	Octyl		0	0.00	*	n		0.00	0.00
165	Octyl		0	0.00	*	n		0.00	0.00
166	DB-1		0	0.01	*	n		0.00	0.00
167	Octyl		0	0.00	*	n		0.00	0.00
168	DB-1		0	0.01	*	n		0.00	0.00
169	Octyl		0	0.01	*	n		0.00	0.00
170	Octyl		0	0.01	*	n		0.04	0.02
171	DB-1		0	0.01	*	n		0.00	0.00
172	Octyl		0	0.01	*	n		0.00	0.00
173	DB-1		0	0.01	*	n		0.00	0.00
174	Octyl		0.017	0.01	1.23	n		0.04	0.02
175	Octyl		0	0.01	*	n		0.00	0.00
176	Octyl		0	0.01	*	n		0.00	0.00
177	Octyl		0	0.01	*	n		0.00	0.00
178	Octyl		0	0.01	*	n		0.00	0.00
179	Octyl		0.018	0.01	0.57	n		0.00	0.00
180	DB-1		0.073	0.01	0.95	y		0.07	0.03
181	Octyl		0	0.01	*	n		0.00	0.00
182	Octyl		0	0.01	*	n		0.00	0.00
183	Octyl		0.014	0.01	0.78	n		0.00	0.00
184	Octyl		0	0.01	*	n		0.00	0.00
185	Octyl		0	0.01	*	n		0.00	0.00
186	Octyl		0	0.01	*	n		0.00	0.00
187	Octyl		0.016	0.01	0.25	n		0.00	0.00
188	Octyl		0	0.01	*	n		0.00	0.00
189	Octyl		0	0.02	*	n		0.00	0.00
190	Octyl		0	0.01	*	n		0.00	0.00

Table A2. (continued) Aroclor 1232: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Frai
							wt %	MS	ECD
191	Octyl		0	0.01	*	n		0.00	0.00
192	Octyl		0	0.01	*	n		0.00	0.00
193	DB-1		0	0.01	*	n		0.00	0.00
194	Octyl		0	0.02	*	n		0.01	0.01
195	Octyl		0	0.02	*	n		0.00	0.00
196	Octyl		0	0.02	*	n		0.00	0.00
197	Octyl		0	0.01	*	n		0.00	0.00
198	DB-1		0	0.01	*	n		0.00	0.00
199	DB-1		0	0.01	*	n		0.02	0.01
200	Octyl		0	0.01	*	n		0.00	0.00
201	Octyl		0	0.01	*	n		0.00	0.00
202	Octyl		0	0.01	*	n		0.00	0.00
203	Octyl		0	0.02	*	n		0.01	0.00
204	Octyl		0	0.01	*	n		0.00	0.00
205	Octyl		0	0.02	*	n		0.00	0.00
206	Octyl		0	0.05	*	n		0.12	IS
207	Octyl		0	0.03	*	n		0.01	0.00
208	Octyl		0	0.03	*	n		0.05	IS
209	Octyl		0	0.02	*	n		0.00	

Homologue Totals

Cl-1	28.45 wt %
Cl-2	21.56 wt %
Cl-3	24.73 wt %
Cl-4	16.95 wt %
Cl-5	2.37 wt %
Cl-6	0.32 wt %
Cl-7	0.14 wt %
Cl-8	0.00 wt %
Cl-9	0.00 wt %
Cl-10	0.00 wt %

94.51 wt %

Table A3. Aroclor 1016: Congener concentrations (wt%) and comparison to published values

(Refer to footnotes for table 15 for explanation of headings)

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL wt %	RA wt %	RA? wt %	S.P.D.	G.Frame	G.Fram
							MS wt %	ECD wt %	
1	Octyl		0.731	0.00	3.06	y		0.54	0.66
2	Octyl		0.037	0.00	2.84	y		0.03	
3	Octyl		0.222	0.00	3.16	y		0.14	
4	Octyl		4.279	0.07	1.45	y	3.89	4.11	1.10
5	Octyl		0.244	0.06	1.20	n	0.13	0.17	0.91
6	Octyl		1.963	0.05	1.45	y	1.83	1.42	0.91
7	Octyl		0.388	0.05	1.25	n	0.60	0.25	0.61
8	Octyl		9.79	0.05	1.48	y	10.80	7.52	1.12
9	Octyl		0.751	0.05	1.35	y	0.95	0.50	0.77
10	Octyl		0.256	0.05	1.08	n	0.37	0.14	0.64
11	Octyl		0.02	0.06	3.11	n		0.02	
12	Octyl	12+13	see 13	0.06	1.37	y		0.06	0.35
13	Octyl	12+13	0.447	0.06	1.37	y		0.21	0.67
14	Octyl		0.007	0.06	0.13	n			
15	Octyl		2.904	0.06	1.46	y	2.90	2.31	0.86
16	Octyl		5.039	0.00	0.95	y	2.86	3.81	0.93
17	Octyl		5.034	0.00	0.94	y	3.84	4.01	1.01
18	DB-1		11.732	0.00	0.99	y	9.03	12.35	1.34
19	Octyl		1.244	0.00	0.96	y	0.96	1.00	0.82
20	Octyl	28+20	see 28	0.01	1.03	y	1.00	0.69	0.90
21	Octyl	21+33	see 33	0.01	1.02	y			
22	Octyl		4.154	0.01	1.02	y	4.80	3.37	0.99
23	Octyl		0.02	0.01	0.78	n		0.01	0.19
24	Octyl		0.185	0.00	0.95	y	0.30	0.14	0.54
25	Octyl		0.858	0.01	0.99	y	1.19	0.69	0.67
26	DB-1		1.492	0.02	0.99	y	1.92	1.58	0.81
27	Octyl		0.673	0.00	0.97	y	0.47	0.56	0.73
28	Octyl	28+20	11.42	0.01	1.03	y	8.71	8.14	1.04
29	DB-1		0.106	0.02	1.13	y	0.19	0.09	0.73
30	DB-1		0.005	0.00	3.55	n		0.01	0.37
31	Octyl		10.773	0.01	1.03	y	6.40	8.85	1.25
32	Octyl		2.792	0.01	1.02	y	1.34	2.24	0.85
33	Octyl	21+33	7.592	0.01	1.02	y	6.25	5.95	0.99
34	Octyl		0.044	0.01	1.05	y	0.12	0.04	0.54
35	Octyl		0.127	0.01	0.97	y	0.08	0.06	0.79

Table A3. (continued) Aroclor 1016: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn. wt %	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							MS wt %	wt %	ECD wt %
36	Octyl		0.001	0.01	0.65	n			
37	Octyl		2.549	0.01	1.02	y	0.30	1.01	1.03
38	Octyl		0.005	0.01	1.69	n			
39	Octyl		0	0.01	*	n			
40	DB-1		1.211	0.03	0.78	y	0.96	0.65	0.60
41	Octyl		0.954	0.00	0.74	y	2.24	0.62	0.76
42	Octyl		1.672	0.00	0.75	y	0.55	1.37	0.83
43	Octyl		0.299	0.00	0.71	y		0.27	0.70
44	DB-1		7.163	0.00	0.77	y	3.50	4.18	0.93
45	DB-1		1.824	0.00	0.77	y	1.66	1.23	0.91
46	Octyl		0.532	0.00	0.72	y	0.70	0.55	0.88
47	DB-1		1.885	0.00	0.70	y	1.11	1.25	0.94
48	Octyl		1.747	0.00	0.74	y	0.98	1.54	0.80
49	Octyl	69+49	3.349	0.00	0.75	y	4.31	3.66	1.04
50	DB-1		0.035	0.00	0.83	y		0.04	
51	DB-1		0.521	0.00	0.75	y	0.36	0.23	
52	Octyl		5.051	0.00	0.74	y	4.46	4.14	0.90
53	DB-1		1.501	0.00	0.77	y	0.55	0.87	0.77
54	Octyl		0.022	0.00	0.81	y		0.02	
55	Octyl		0.026	0.01	0.50	n		0.01	0.19
56	Octyl		0.126	0.01	0.78	y	0.10	0.09	0.61
57	Octyl		0.029	0.01	0.91	n		0.01	0.36
58	Octyl		0	0.01	*	n			
59	Octyl	59+62+75	0.597	0.00	0.75	y	0.29	0.33	0.61
60	Octyl		0.062	0.01	0.84	y	0.07		
61	DB-1	74+61	see 74	0.03	0.77	y			
62	DB-1	65+62	0.015	0.01	1.01	n			
63	Octyl		0.128	0.01	0.76	y	0.15	0.06	0.83
64	Octyl		2.553	0.00	0.75	y	1.80	1.87	0.76
65	DB-1	65+62	see 62	0.01	1.01	n			
66	Octyl		0.934	0.01	0.77	y	1.60	0.35	0.66
67	Octyl		0.145	0.01	0.81	y	0.27	0.06	0.63
68	Octyl		0.009	0.01	1.02	n			
69	Octyl	69+49	see 49	0.00	0.75	y		0.01	
70	DB-1		1.94	0.02	0.77	y	1.20	0.48	0.62
71	Octyl	40+71	see 40	0.00	0.76	y		1.11	1.12
72	Octyl		0.025	0.01	0.84	y		0.01	0.63
73	Octyl		0	0.00	*	n		0.01	
74	DB-1	74+61	2.14	0.03	0.77	y	0.89	0.32	0.74

Table A3. (continued) Aroclor 1016: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL wt %	RA wt %	RA? y	S.P.D. wt %	G.Frame MS wt %	G.Fram ECD wt %
							wt %	wt %	wt %
75	Octyl	59+62+75	see 59	0.00	0.75	y	0.08		
76	Octyl	61+70+74+76	see 70	0.02	0.76	y			
77	Octyl		0.002	0.02	0.24	n		0.00	
78	Octyl		0	0.01	*	n			
79	Octyl		0	0.01	*	n			
80	Octyl		0	0.01	*	n			
81	Octyl		0	0.01	*	n			
82	Octyl		0.002	0.00	0.50	n		0.00	
83	DB-1	83+112	0	0.02	*	n			
84	Octyl		0.142	0.00	1.51	y	0.14	0.05	0.64
85	Octyl	117+116+85	0	0.00	*	n		0.01	0.25
86	DB-1		0	0.02	*	n			
87	Octyl	108+119+86+97+1 25+87	0.002	0.00	2.49	n		0.01	0.29
88	DB-1		0	0.02	*	n			
89	Octyl		0.012	0.00	0.65	n			
90	Octyl	113+90+101	see 101	0.00	1.65	y			
91	DB-1		0.23	0.02	1.56	y	0.15	0.06	0.45
92	Octyl		0.027	0.00	1.84	n		0.02	
93	Octyl	100+93	0.028	0.00	2.10	n			
94	Octyl		0.019	0.00	1.54	y		0.01	0.34
95	Octyl		0.764	0.00	1.64	y	0.55	0.27	0.58
96	Octyl		0.042	0.00	1.65	y		0.03	
97	DB-1		0.004	0.02	0.82	n		0.01	0.23
98	Octyl	102+98	see 102	0.00	1.53	y			
99	Octyl	83+99	0.029	0.00	1.51	y		0.01	0.45
100	DB-1		0.012	0.02	0.82	n			
101	Octyl	113+90+101	0.08	0.00	1.65	y	0.15	0.03	0.41
102	Octyl	102+98	0.105	0.00	1.53	y		0.04	0.47
103	Octyl		0.013	0.00	1.28	n		0.01	
104	Octyl		0	0.00	*	n			
105	Octyl		0.009	0.00	1.56	y		0.00	0.13
106	Octyl		0	0.00	*	n		0.01	
107	Octyl	107+124	see 124	0.00	*	n			
108	DB-1		0	0.01	*	n			
109	Octyl		0	0.00	*	n			
110	Octyl	110+115	0.01	0.00	2.35	n		0.01	0.38
111	Octyl		0	0.00	*	n			
112	Octyl		0	0.00	*	n			

Table A3. (continued) Aroclor 1016: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn. wt %	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							MS wt %	wt %	ECD wt %
113	Octyl	113+90+101	see 101	0.00	1.65	y			
114	Octyl		0	0.00	*	n			
115	Octyl	110+115	see 110	0.00	2.35	n			
116	Octyl	117+116+85	see 85	0.00	*	n			
117	Octyl	117+116+85	see 85	0.00	*	n			
118	Octyl		0.013	0.00	1.36	y		0.01	
119	DB-1		0	0.01	*	n			
120	Octyl		0	0.00	*	n			
121	Octyl		0	0.00	*	n			
122	Octyl		0	0.00	*	n			
123	Octyl		0	0.00	*	n			
124	Octyl	107+124	0	0.00	*	n			
125	Octyl	108+119+86+97+1 25+87	see 97	0.00	2.49	n			
126	Octyl		0	0.00	*	n			
127	Octyl		0	0.00	*	n			
128	DB-1		0	0.00	*	n			
129	DB-1		0	0.00	*	n			
130	Octyl		0	0.00	*	n			
131	Octyl		0	0.00	*	n			
132	Octyl		0	0.00	*	n			
133	Octyl		0	0.00	*	n			
134	Octyl	134+143	0	0.00	*	n			
135	Octyl	151+135	0	0.00	*	n			
136	Octyl		0	0.00	*	n			
137	Octyl		0	0.00	*	n			
138	DB-1	138+163+164	0	0.00	*	n	0.19		
139	Octyl	139+140	0	0.00	*	n			
140	DB-1		0	0.00	*	n			
141	Octyl		0	0.00	*	n			
142	Octyl		0	0.00	*	n			
143	Octyl	134+143	see 134	0.00	*	n			
144	Octyl		0	0.00	*	n			
145	Octyl		0	0.00	*	n			
146	Octyl		0	0.00	*	n			
147	DB-1		0	0.00	*	n			
148	Octyl		0	0.00	*	n			
149	DB-1	139+149	0	0.00	*	n			
150	Octyl		0	0.00	*	n			

Table A3. (continued) Aroclor 1016: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn. wt %	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							MS	wt %	ECD
151	DB-1		0	0.00	*	n			
152	Octyl		0	0.00	*	n			
153	DB-1		0	0.00	*	n			
154	Octyl		0	0.00	*	n			
155	Octyl		0	0.00	*	n			
156	DB-1		0	0.00	*	n			
157	DB-1		0	0.00	*	n			
158	Octyl		0	0.00	*	n			
159	Octyl		0	0.00	*	n			
160	DB-1	158+160	0	0.00	*	n			
161	Octyl		0	0.00	*	n			
162	Octyl		0	0.00	*	n			
163	Octyl	138+163+129+160	see 138	0.00	*	n			
164	Octyl		0	0.00	*	n			
165	Octyl		0	0.00	*	n			
166	DB-1		0	0.00	*	n			
167	Octyl		0	0.00	*	n			
168	DB-1		0	0.00	*	n			
169	Octyl		0	0.00	*	n			
170	Octyl		0	0.00	*	n			
171	DB-1		0	0.00	*	n		0.02	
172	Octyl		0	0.00	*	n			
173	DB-1		0	0.00	*	n			
174	Octyl		0	0.00	*	n			
175	Octyl		0	0.00	*	n			
176	Octyl		0	0.00	*	n			
177	Octyl		0	0.00	*	n			
178	Octyl		0	0.00	*	n			
179	Octyl		0	0.00	*	n			
180	DB-1		0	0.00	*	n			
181	Octyl		0	0.00	*	n			
182	Octyl		0	0.00	*	n			
183	Octyl		0	0.00	*	n			
184	Octyl		0	0.00	*	n			
185	Octyl		0	0.00	*	n			
186	Octyl		0	0.00	*	n			
187	Octyl		0	0.00	*	n			
188	Octyl		0	0.00	*	n			
189	Octyl		0	0.01	*	n			
190	Octyl		0	0.00	*	n			

Table A3. (continued) Aroclor 1016: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn. wt %	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							MS	wt %	wt %
191	Octyl		0	0.00	*	n			
192	Octyl		0	0.00	*	n			
193	DB-1		0	0.00	*	n			
194	Octyl		0	0.00	*	n			
195	Octyl		0	0.00	*	n			
196	Octyl		0	0.00	*	n			
197	Octyl		0	0.00	*	n			
198	DB-1		0	0.00	*	n			
199	DB-1		0	0.00	*	n			
200	Octyl		0	0.00	*	n			
201	Octyl		0	0.00	*	n			
202	Octyl		0	0.00	*	n			
203	Octyl		0	0.00	*	n			
204	Octyl		0	0.00	*	n			
205	Octyl		0	0.00	*	n			
206	Octyl		0	0.01	*	n			
207	Octyl		0	0.01	*	n			
208	Octyl		0	0.01	*	n		0.01	0.26
209	Octyl		0	0.00	*	n			

Homologue Totals

Cl-1	0.99 wt %
Cl-2	21.05 wt %
Cl-3	65.84 wt %
Cl-4	36.50 wt %
Cl-5	1.54 wt %
Cl-6	0.00 wt %
Cl-7	0.00 wt %
Cl-8	0.00 wt %
Cl-9	0.00 wt %
Cl-10	0.00 wt %

125.92 wt %

Table A4. Aroclor 1242: Congener concentrations (wt%) and comparison to published values

(Refer to footnotes for table 15 for explanation of headings)

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn. wt %	SDL wt %	RA wt %	RA? y	S.P.D. wt %	G.Frame MS wt %	G.Frame ECD wt %
1	Octyl		0.545	0.00	3.08	y		0.54	
2	Octyl		0.028	0.00	3.01	y		0.03	
3	Octyl		0.163	0.00	2.94	y		0.14	
4	Octyl		2.725	0.05	1.44	y	3.01	3.51	3.70
5	Octyl		0.137	0.04	1.30	n	0.06	0.14	0.23
6	Octyl		1.235	0.04	1.47	y	1.38	1.19	1.51
7	Octyl		0.253	0.04	1.30	n	0.60	0.22	0.41
8	Octyl		5.915	0.04	1.47	y	7.65	6.12	6.68
9	Octyl		0.501	0.04	1.43	y	0.54	0.40	0.59
10	Octyl		0.183	0.04	1.01	n	0.20	0.11	0.22
11	Octyl		0.022	0.04	0.82	n		0.01	
12	Octyl	12+13	see 13	0.05	1.30	n		0.05	0.13
13	Octyl	12+13	0.283	0.05	1.30	n		0.19	
14	Octyl		0.002	0.04	0.12	n			0.08
15	Octyl		1.842	0.04	1.49	y	1.51	1.74	2.62
16	Octyl		3.128	0.00	0.95	y	2.01	3.10	3.73
17	Octyl		3.158	0.00	0.94	y	2.88	3.22	3.33
18	DB-1		7.334	0.00	1.00	y	6.28	9.24	8.03
19	Octyl		0.804	0.00	0.94	y	0.53	0.80	1.07
20	Octyl	28+20	see 28	0.01	1.01	y	0.29	0.51	0.45
21	Octyl	21+33	see 33	0.01	1.03	y			
22	Octyl		2.637	0.01	1.03	y	3.41	2.48	2.94
23	Octyl		0.011	0.01	1.10	y		0.01	0.05
24	Octyl		0.113	0.00	0.94	y	0.22	0.11	0.21
25	Octyl		0.535	0.01	1.05	y	0.79	0.54	1.02
26	DB-1		0.911	0.01	1.01	y	1.33	1.17	1.57
27	Octyl		0.415	0.00	0.94	y	0.28	0.46	0.56
28	Octyl	28+20	6.729	0.01	1.01	y	6.52	6.08	5.82
29	DB-1		0.062	0.01	1.17	y	0.10	0.08	0.08
30	DB-1		0.005	0.00	1.85	n		0.00	
31	Octyl		6.56	0.01	1.02	y	4.59	6.34	6.04
32	Octyl		1.883	0.01	1.03	y	0.88	1.70	2.29
33	Octyl	21+33	4.417	0.01	1.03	y	4.79	4.31	5.08
34	Octyl		0.027	0.01	1.16	y	0.05	0.03	0.06
35	Octyl		0.084	0.01	1.09	y	0.11	0.06	0.13

Table A4. (continued) Aroclor 1242: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Frame
								MS	ECD
			wt %	wt %			wt %	wt %	wt %
36	Octyl		0.001	0.01	3.50	n		0.04	
37	Octyl		1.83	0.02	1.07	y	0.27	1.78	1.81
38	Octyl		0.003	0.01	1.58	n			
39	Octyl		0.026	0.01	1.07	y			
40	DB-1		0.734	0.02	0.79	y	0.89	0.78	1.08
41	Octyl		0.59	0.00	0.73	y	1.86	0.59	0.83
42	Octyl		1.083	0.00	0.76	y	0.83	1.13	1.46
43	Octyl		0.205	0.00	0.75	y		0.18	0.30
44	DB-1		4.411	0.00	0.77	y	3.20	3.32	3.86
45	DB-1		1.134	0.00	0.75	y	1.16	0.92	1.43
46	Octyl		0.347	0.00	0.73	y	0.49	0.41	0.51
47	DB-1		1.058	0.00	0.74	y	0.94	0.96	1.10
48	Octyl		1.188	0.00	0.79	y	0.82	1.16	1.55
49	Octyl	69+49	2.343	0.00	0.75	y	3.60	2.91	2.94
50	DB-1		0.024	0.00	1.12	n		0.02	
51	DB-1		0.315	0.00	0.69	y	0.23	0.17	0.60
52	Octyl		3.639	0.00	0.75	y	4.04	3.22	3.54
53	DB-1		0.923	0.00	0.75	y	0.64	0.66	0.73
54	Octyl		0.012	0.00	0.54	n		0.01	
55	Octyl		0.109	0.02	0.86	y		0.08	0.14
56	Octyl		1.617	0.02	0.75	y	1.60	1.28	1.82
57	Octyl		0.024	0.02	0.60	n		0.03	0.06
58	Octyl		0	0.02	*	n		0.01	
59	Octyl	59+62+75	0.388	0.00	0.73	y	0.34	0.27	0.47
60	Octyl		1.108	0.02	0.77	y	1.33	0.91	1.42
61	DB-1	74+61	see 74	0.03	0.77	y			
62	DB-1	65+62	0	0.00	*	n			0.03
63	Octyl		0.155	0.02	0.82	y	0.23	0.16	0.25
64	Octyl		1.737	0.00	0.75	y	1.64	1.68	2.25
65	DB-1	65+62	see 62	0.00	*	n			
66	Octyl		2.876	0.02	0.77	y	1.66	3.12	3.68
67	Octyl		0.149	0.01	0.75	y	0.41	0.12	0.23
68	Octyl		0.005	0.01	0.58	n		0.00	0.02
69	Octyl	69+49	see 49	0.00	0.75	y	0.11	0.01	
70	DB-1		3.73	0.02	0.76	y	3.89	3.09	3.82
71	Octyl	40+71	see 40	0.00	0.75	y		0.85	1.07
72	Octyl		0.015	0.02	0.91	n		0.02	0.05
73	Octyl		0	0.00	*	n		0.00	
74	DB-1	74+61	3.407	0.03	0.77	y	2.17	1.79	2.25

Table A4. (continued) Aroclor 1242: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame MS	G.Frame ECD
			wt %	wt %			wt %	wt %	wt %
75	Octyl	59+62+75	see 59	0.00	0.73	y	0.11	0.90	0.08
76	Octyl	61+70+74+ 76	see 70	0.02	0.77	y		0.06	
77	Octyl		0.296	0.02	0.72	y	0.45	0.23	0.37
78	Octyl		0	0.02	*	n			
79	Octyl		0.015	0.01	0.54	n			
80	Octyl		0	0.01	*	n			
81	Octyl		0.012	0.02	1.13	n		0.02	0.03
82	Octyl		0.245	0.00	1.64	y	0.44	0.26	0.32
83	DB-1	83+112	0.079	0.02	1.74	y	0.12	0.07	0.13
84	Octyl		0.433	0.00	1.53	y	0.72	0.34	0.76
85	Octyl	117+116+85	0.27	0.00	1.54	y	0.53	0.28	0.42
86	DB-1		0	0.02	*	n		0.03	0.02
87	Octyl	108+119+86 +97+125+8 7	0.508	0.00	1.44	y	0.77	0.45	0.65
88	DB-1		0.009	0.02	1.20	n		0.01	
89	Octyl		0.046	0.00	1.81	n		0.05	0.07
90	Octyl	113+90+101	see 101	0.00	1.54	y	0.32	0.04	0.02
91	DB-1		0.245	0.02	1.75	y	0.17	0.21	0.33
92	Octyl		0.181	0.00	1.60	y	0.25	0.12	0.28
93	Octyl	100+93	0.018	0.00	0.83	n		0.02	0.13
94	Octyl		0.012	0.00	1.44	y		0.01	0.07
95	Octyl		0.866	0.00	1.50	y	2.87	0.64	0.91
96	Octyl		0.033	0.00	1.57	y		0.03	0.12
97	DB-1		0.481	0.02	1.51	y	0.65	0.38	0.60
98	Octyl	102+98	see 102	0.00	1.66	y			
99	Octyl	83+99	0.656	0.00	1.44	y	0.86	0.39	0.67
100	DB-1		0.009	0.02	0.47	n			
101	Octyl	113+90+101	1.002	0.00	1.54	y	1.33	0.67	0.99
102	Octyl	102+98	0.086	0.00	1.66	y		0.07	0.10
103	Octyl		0.005	0.00	4.89	n		0.01	0.02
104	Octyl		0	0.00	*	n			
105	Octyl		0.511	0.01	1.48	y	0.86	0.41	0.61
106	Octyl		0	0.01	*	n			
107	Octyl	107+124	see 124	0.01	1.56	y			
108	DB-1		0	0.01	*	n			
109	Octyl		0.069	0.01	1.73	y	0.07	0.06	0.12
110	Octyl	110+115	1.142	0.00	1.56	y	1.53	0.77	1.13
111	Octyl		0	0.00	*	n			0.45

Table A4. (continued) Aroclor 1242: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Frame
								MS	ECD
			wt %	wt %			wt %	wt %	wt %
112	Octyl		0	0.00	*	n		0.01	
113	Octyl	113+90+101	see 101	0.00	1.54	y			0.15
114	Octyl		0.041	0.01	1.93	n		0.03	0.05
115	Octyl	110+115	see 110	0.00	1.56	y		0.05	0.07
116	Octyl	117+116+85	see 85	0.00	1.54	y			
117	Octyl	117+116+85	see 85	0.00	1.54	y		0.03	0.06
118	Octyl		0.958	0.01	1.54	y	1.62	0.69	0.99
119	DB-1		0.024	0.01	2.01	n	0.05	0.02	0.05
120	Octyl		0	0.00	*	n			
121	Octyl		0	0.00	*	n			0.09
122	Octyl		0.024	0.01	1.81	n		0.02	0.08
123	Octyl		0.027	0.01	1.72	y		0.03	0.04
124	Octyl	107+124	0.04	0.01	1.56	y		0.04	0.32
125	Octyl	108+119+86	see 97	0.00	1.44	y			
		+97+125+8		7					
126	Octyl		0	0.01	*	n			
127	Octyl		0	0.01	*	n			
128	DB-1		0.077	0.01	1.50	n		0.04	0.06
129	DB-1		0.018	0.01	1.28	y		0.01	0.08
130	Octyl		0.028	0.00	0.92	n		0.01	0.03
131	Octyl		0.004	0.00	1.25	y			0.01
132	Octyl		0.138	0.00	1.21	y	0.30	0.06	0.07
133	Octyl		0	0.00	*	n			0.01
134	Octyl	134+143	0.045	0.01	1.04	n			
135	Octyl	151+135	0.104	0.00	1.04	n	0.08	0.01	
136	Octyl		0.048	0.00	1.35	y	0.07	0.01	0.04
137	Octyl		0.029	0.00	1.22	y		0.01	0.03
138	DB-1	138+163+16	0.366	0.01	1.17	y	0.54	0.12	0.18
		4							
139	Octyl	139+140	0.011	0.00	0.93	n			
140	DB-1		0	0.01	*	n			
141	Octyl		0.065	0.00	1.16	y		0.02	0.05
142	Octyl		0	0.00	*	n			
143	Octyl	134+143	see 134	0.01	1.04	n			
144	Octyl		0.018	0.00	1.03	n			0.13
145	Octyl		0	0.00	*	n			
146	Octyl		0.039	0.00	1.29	y		0.01	0.03
147	DB-1		0.01	0.01	1.32	y			
148	Octyl		0	0.00	*	n			

Table A4. (continued) Aroclor 1242: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Frame
							wt %	MS	ECD
149	DB-1	139+149	0.249	0.01	1.23	y	0.63	0.06	0.12
150	Octyl		0	0.00	*	n			
151	DB-1		0.048	0.01	0.92	n		0.01	
152	Octyl		0	0.00	*	n			0.32
153	DB-1		0.235	0.01	1.20	y	0.68	0.08	0.17
154	Octyl		0	0.00	*	n			
155	Octyl		0	0.00	*	n			
156	DB-1		0.048	0.01	0.82	n	0.09	0.02	0.06
157	DB-1		0.013	0.01	1.54	n		0.01	0.02
158	Octyl		0.055	0.00	1.26	y		0.02	0.03
159	Octyl		0	0.00	*	n			
160	DB-1	158+160	0.004	0.01	1.57	n			0.03
161	Octyl		0	0.00	*	n			
162	Octyl		0	0.00	*	n			
163	Octyl	138+163+12 9+160	see 138	0.00	1.20	y			
164	Octyl		0.028	0.00	1.49	n		0.03	0.08
165	Octyl		0	0.00	*	n			
166	DB-1		0	0.00	*	n			
167	Octyl		0.017	0.00	2.44	n		0.01	0.02
168	DB-1		0	0.00	*	n		0.00	
169	Octyl		0	0.00	*	n			
170	Octyl		0.029	0.00	0.95	y	0.11	0.01	0.02
171	DB-1		0.006	0.00	2.08	n	0.05	0.02	0.06
172	Octyl		0	0.00	*	n			
173	DB-1		0	0.00	*	n			
174	Octyl		0.013	0.00	0.51	n			0.02
175	Octyl		0	0.00	*	n			
176	Octyl		0.002	0.00	0.78	n			
177	Octyl		0.007	0.00	2.69	n			
178	Octyl		0	0.00	*	n			
179	Octyl		0.005	0.00	0.65	n			
180	DB-1		0.043	0.00	1.19	y	0.06	0.01	0.03
181	Octyl		0	0.00	*	n			
182	Octyl		0	0.00	*	n			
183	Octyl		0.008	0.00	0.56	n			
184	Octyl		0	0.00	*	n			
185	Octyl		0	0.00	*	n			
186	Octyl		0	0.00	*	n			
187	Octyl		0.012	0.00	1.31	n			

Table A4. (continued) Aroclor 1242: Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn. wt %	SDL wt %	RA wt %	RA? *	S.P.D. wt %	G.Frame MS wt %	G.Frame ECD wt %
188	Octyl		0	0.00	*	n			
189	Octyl		0	0.01	*	n			
190	Octyl		0	0.00	*	n			
191	Octyl		0	0.00	*	n			
192	Octyl		0	0.00	*	n			
193	DB-1		0	0.00	*	n			
194	Octyl		0	0.01	*	n			
195	Octyl		0	0.00	*	n		0.12	
196	Octyl		0	0.00	*	n			
197	Octyl		0	0.00	*	n			
198	DB-1		0	0.01	*	n			
199	DB-1		0	0.01	*	n			
200	Octyl		0	0.00	*	n			
201	Octyl		0	0.00	*	n		0.05	
202	Octyl		0	0.00	*	n			
203	Octyl		0	0.00	*	n			
204	Octyl		0	0.00	*	n			
205	Octyl		0	0.00	*	n			
206	Octyl		0	0.02	*	n		0.04	0.08
207	Octyl		0	0.01	*	n			0.01
208	Octyl		0	0.01	*	n		0.02	0.04
209	Octyl		0	0.01	*	n			

Homologue Totals

Cl-1	0.74 wt %
Cl-2	13.10 wt %
Cl-3	40.64 wt %
Cl-4	33.68 wt %
Cl-5	8.02 wt %
Cl-6	1.70 wt %
Cl-7	0.13 wt %
Cl-8	0.00 wt %
Cl-9	0.00 wt %
Cl-10	0.00 wt %

98.00 wt %

Table A5. Aroclor 1248 : Congener concentrations (wt%) and comparison to published values

(Refer to footnotes for table 15 for explanation of headings)

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL wt %	RA wt %	RA? wt %	S.P.D. MS wt %	G.Frame wt %	G.Fram wt %
1	Octyl		0.013	0.00	2.57	n	0.71	0.14	
2	Octyl		0	0.00	*	n	0.00	0.00	
3	Octyl		0.006	0.00	6.44	n	0.00	0.02	
4	Octyl		0.111	0.00	0.85	n	0.00	0.53	
5	Octyl		0.001	0.00	2.45	n	0.00	0.00	
6	Octyl		0.029	0.00	0.80	n	0.21	0.21	
7	Octyl		0.008	0.00	0.40	n	0.05	0.05	
8	Octyl		0.46	0.00	1.47	y	1.14	1.16	
9	Octyl		0.008	0.00	0.71	n	0.07	0.07	
10	Octyl		0.014	0.00	0.04	n	0.00	0.06	
11	Octyl		0	0.00	*	n	0.00	0.00	
12	Octyl	12+13	see 13	0.00	0.76	n	0.00	0.01	
13	Octyl	12+13	0.005	0.00	0.76	n	0.00	0.01	
14	Octyl		0	0.00	*	n	0.00	0.00	
15	Octyl		0.182	0.00	1.30	n	0.00	0.30	
16	Octyl		1.338	0.00	0.95	y	1.40	1.17	
17	Octyl		1.414	0.00	0.97	y	1.29	1.27	
18	DB-1		4.178	0.00	1.00	y	4.36	4.58	
19	Octyl		0.252	0.00	1.02	y	0.30	0.30	
20	Octyl	28+20	see 28	0.00	1.02	y	@28	@33	
21	Octyl	21+33	see 33	0.00	1.03	y	0.00	0.00	
22	Octyl		1.842	0.00	1.02	y	1.54	1.50	
23	Octyl		0.006	0.00	0.60	n	0.00	0.00	
24	Octyl		0.002	0.00	1.99	n	0.02	0.01	
25	Octyl		0.107	0.00	1.15	y	0.00	0.16	
26	DB-1		0.313	0.02	1.02	y	0.57	0.56	
27	Octyl		0.133	0.00	0.90	y	0.18	0.18	
28	Octyl	28+20	6.256	0.00	1.02	y	3.44	3.36	
29	DB-1		0.008	0.02	1.31	n	0.00	0.01	
30	DB-1		0	0.00	*	n	0.00	0.00	
31	Octyl		6.212	0.00	1.02	y	4.36	4.53	
32	Octyl		1.226	0.00	1.04	y	1.10	1.18	
33	Octyl	21+33	2.879	0.00	1.03	y	2.59	2.51	
34	Octyl		0.008	0.00	1.83	n	0.00	0.00	
35	Octyl		0.002	0.00	2.21	n	0.00	0.00	

Table A5. (continued) Aroclor 1248 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							wt %	wt %	wt %
36	Octyl		0	0.00	*	n		0.00	0.00
37	Octyl		1.305	0.00	1.00	y		@64	0.76
38	Octyl		0.005	0.00	0.82	n		0.00	0.00
39	Octyl		0	0.00	*	n		0.00	0.00
40	DB-1		1.221	0.03	0.73	y		3.11	1.21
41	Octyl		0.75	0.00	0.70	y		0.89	0.89
42	Octyl		1.83	0.00	0.73	y		1.91	1.91
43	Octyl		0.263	0.00	0.76	y		0.29	0.29
44	DB-1		7.793	0.00	0.75	y		5.91	5.95
45	DB-1		1.316	0.00	0.76	y		1.39	1.30
46	Octyl		0.476	0.00	0.74	y		0.59	0.55
47	DB-1		2.566	0.00	0.73	y		1.29	1.40
48	Octyl		1.673	0.00	0.73	y		1.72	1.73
49	Octyl	69+49	3.858	0.00	0.75	y		4.04	4.24
50	DB-1		0.02	0.00	0.72	y		0.00	0.00
51	DB-1		0.435	0.00	0.78	y		0.00	0.28
52	Octyl		6.235	0.00	0.74	y		5.94	6.22
53	DB-1		1.318	0.00	0.77	y		1.45	1.04
54	Octyl		0.015	0.00	0.78	y		0.00	0.00
55	Octyl		0.097	0.00	0.83	y		0.14	0.07
56	Octyl		3.226	0.00	0.77	y		2.83	2.83
57	Octyl		0.026	0.00	0.64	n		0.00	0.01
58	Octyl		0	0.00	*	n		0.00	0.00
59	Octyl	59+62+75	0.471	0.00	0.72	y		0.49	0.49
60	Octyl		2.368	0.00	0.78	y		1.90	1.90
61	DB-1	74+61	see 74	0.04	0.75	y		0.00	0.00
62	DB-1	65+62	0.007	0.01	1.57	n		0.00	0.00
63	Octyl		0.252	0.00	0.76	y		0.31	0.28
64	Octyl		3.342	0.00	0.74	y	3.35	3.35	
65	DB-1	65+62	see 62	0.01	1.57	n		0.00	0.00
66	Octyl		6.417	0.00	0.78	y		4.98	5.18
67	Octyl		0.123	0.00	0.72	y		0.25	0.18
68	Octyl		0.008	0.00	0.47	n		0.00	0.00
69	Octyl	69+49	see 49	0.00	0.75	y		0.00	0.00
70	DB-1		8.014	0.02	0.76	y		6.00	5.50
71	Octyl	40+71	see 40	0.00	0.73	y		0.00	@40
72	Octyl		0.019	0.00	0.78	y		0.00	0.00
73	Octyl		0	0.00	*	n		0.00	0.00

Table A5. (continued) Aroclor 1248 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							wt %	wt %	wt %
74	DB-1	74+61	7.688	0.04	0.75	y		3.03	2.94
75	Octyl	59+62+75	see 59	0.00	0.72	y		0.10	0.05
76	Octyl	61+70+74+76	see 70	0.00	0.77	y		0.00	0.00
77	Octyl		0.609	0.00	0.76	y		0.43	0.36
78	Octyl		0	0.00	*	n		0.00	0.00
79	Octyl		0	0.00	*	n		0.00	0.00
80	Octyl		0.002	0.00	0.34	n		0.00	0.00
81	Octyl		0.041	0.00	0.66	y		0.00	0.00
82	Octyl		0.552	0.00	1.55	y		0.84	0.78
83	DB-1	83+112	0.125	0.01	1.37	y		0.00	0.24
84	Octyl		0.868	0.00	1.62	y		1.28	1.28
85	Octyl	117+116+85	0.731	0.00	1.45	y		1.04	0.96
86	DB-1		0	0.01	*	n		0.00	0.00
87	Octyl	108+119+86+97+125 +87	0.966	0.00	1.55	y		1.59	1.52
88	DB-1		0	0.01	*	n		0.00	0.00
89	Octyl		0.11	0.00	1.29	n		0.15	0.14
90	Octyl	113+90+101	see 101	0.00	1.55	y		0.00	0.00
91	DB-1		0.457	0.01	1.50	y		0.00	0.33
92	Octyl		0.268	0.00	1.54	y		0.53	0.53
93	Octyl	100+93	0.045	0.00	1.52	y		0.00	0.00
94	Octyl		0.022	0.00	2.67	n		0.00	0.00
95	Octyl		1.473	0.00	1.58	y		2.05	2.12
96	Octyl		0.057	0.00	1.50	y		0.00	0.04
97	DB-1		0.93	0.01	1.56	y		1.51	1.17
98	Octyl	102+98	see 102	0.00	1.58	y		0.00	0.00
99	Octyl	83+99	1.603	0.00	1.53	y		1.57	1.45
100	DB-1		0.018	0.01	0.64	n		0.00	0.00
101	Octyl	113+90+101	1.738	0.00	1.55	y		2.34	2.21
102	Octyl	102+98	0.178	0.00	1.58	y		0.27	0.27
103	Octyl		0.014	0.00	1.83	n		0.00	0.00
104	Octyl		0	0.00	*	n		0.00	0.00
105	Octyl		1.308	0.02	1.56	y		1.46	1.32
106	Octyl		0	0.02	*	n		0.00	0.00
107	Octyl	107+124	see 124	0.02	1.50	y		0.08	0.04
108	DB-1		0	0.01	*	n			
109	Octyl		0.133	0.02	1.58	y		0.21	0.18
110	Octyl	110+115	2.305	0.00	1.60	y		2.79	2.67
111	Octyl		0	0.00	*	n		0.00	0.00

Table A5. (continued) Aroclor 1248 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							wt %	wt %	wt %
112	Octyl		0	0.00	*	n		0.00	0.00
113	Octyl	113+90+101	see 101	0.00	1.55	y		0.00	0.00
114	Octyl		0.108	0.02	1.52	y		0.12	0.11
115	Octyl	110+115	see 110	0.00	1.60	y		0.12	0.12
116	Octyl	117+116+85	see 85	0.00	1.45	y		0.00	0.00
117	Octyl	117+116+85	see 85	0.00	1.45	y		0.10	0.05
118	Octyl		1.975	0.03	1.50	y		2.32	2.18
119	DB-1		0.048	0.01	1.49	y		0.00	0.03
120	Octyl		0	0.00	*	n		0.00	0.00
121	Octyl		0	0.00	*	n		0.00	0.00
122	Octyl		0.052	0.03	1.46	y		0.05	0.03
123	Octyl		0.052	0.02	1.31	n		0.08	0.04
124	Octyl	107+124	0.067	0.02	1.50	y		0.00	0.04
125	Octyl	108+119+86+97+125 +87	see 97	0.00	1.55	y		0.00	0.00
126	Octyl		0	0.03	*	n		0.00	0.00
127	Octyl		0	0.03	*	n		0.00	0.00
128	DB-1		0.056	0.01	1.15	y		0.13	0.13
129	DB-1		0.023	0.01	1.52	n		0.00	0.00
130	Octyl		0.024	0.00	1.32	y		0.04	0.02
131	Octyl		0	0.00	*	n		0.08	0.04
132	Octyl		0.141	0.00	1.17	y		0.20	0.18
133	Octyl		0	0.00	*	n		0.00	0.00
134	Octyl	134+143	0.038	0.00	0.83	n		0.00	0.00
135	Octyl	151+135	0.229	0.00	1.30	y		0.00	0.00
136	Octyl		0.051	0.00	1.33	y		0.48	0.05
137	Octyl		0.022	0.00	0.95	n		0.00	0.00
138	DB-1	138+163+164	0.423	0.00	1.32	y		0.53	0.46
139	Octyl	139+140	0.006	0.00	0.97	n		0.00	0.00
140	DB-1		0	0.01	*	n		0.00	0.00
141	Octyl		0.089	0.00	1.46	n		0.10	0.08
142	Octyl		0	0.00	*	n		0.00	0.00
143	Octyl	134+143	see 134	0.00	0.83	n		0.00	0.00
144	Octyl		0.02	0.00	1.71	n		0.05	0.03
145	Octyl		0	0.00	*	n		0.00	0.00
146	Octyl		0.039	0.00	1.11	y		0.13	0.08
147	DB-1		0	0.00	*	n		0.00	0.00
148	Octyl		0	0.00	*	n		0.00	0.00
149	DB-1	139+149	0.278	0.00	1.21	y		0.35	0.32

Table A5. (continued) Aroclor 1248 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							wt %	wt %	wt %
150	Octyl		0	0.00	*	n		0.00	0.00
151	DB-1		0.084	0.01	1.19	y		0.05	0.07
152	Octyl		0	0.00	*	n		0.00	0.00
153	DB-1		0.313	0.00	1.30	y		0.40	0.34
154	Octyl		0	0.00	*	n		0.00	0.00
155	Octyl		0	0.00	*	n		0.00	0.00
156	DB-1		0.046	0.01	1.08	y		0.09	0.09
157	DB-1		0	0.01	*	n		0.00	0.00
158	Octyl		0.048	0.00	1.36	y		0.07	0.04
159	Octyl		0	0.00	*	n		0.00	0.00
160	DB-1	158+160	-0.006	0.00	1.14	y		0.00	0.00
161	Octyl		0	0.00	*	n		0.00	0.00
162	Octyl		0	0.00	*	n		0.00	0.00
163	Octyl	138+163+129+160	see 138	0.00	1.29	y		0.00	0.00
164	Octyl		0.022	0.00	1.35	y		0.07	0.04
165	Octyl		0	0.00	*	n		0.00	0.00
166	DB-1		0	0.00	*	n		0.00	0.00
167	Octyl		0.013	0.00	0.83	n		0.02	0.01
168	DB-1		0	0.00	*	n		0.00	0.00
169	Octyl		0	0.00	*	n		0.00	0.00
170	Octyl		0.162	0.00	0.93	y		0.06	0.03
171	DB-1		0	0.00	*	n		0.00	0.00
172	Octyl		0.027	0.00	0.92	y		0.00	0.00
173	DB-1		0.003	0.00	1.22	n		0.00	0.00
174	Octyl		0.114	0.00	0.87	n		0.11	0.05
175	Octyl		0	0.00	*	n		0.00	0.00
176	Octyl		0.009	0.00	0.86	n		0.00	0.00
177	Octyl		0.067	0.00	1.00	y		0.04	0.02
178	Octyl		0.021	0.00	1.51	n		0.00	0.00
179	Octyl		0.031	0.00	1.07	y		0.00	0.01
180	DB-1		0.354	0.00	1.05	y		0.21	0.10
181	Octyl		0	0.00	*	n		0.00	0.00
182	Octyl		0	0.00	*	n		0.00	0.00
183	Octyl		0.061	0.00	1.00	y		0.00	0.00
184	Octyl		0	0.00	*	n		0.00	0.00
185	Octyl		0.01	0.00	1.27	n		0.00	0.00
186	Octyl		0	0.00	*	n		0.00	0.00
187	Octyl		0.099	0.00	1.06	y		0.13	0.10
188	Octyl		0	0.00	*	n		0.00	0.00
189	Octyl		0	0.01	*	n		0.00	0.00

Table A5. (continued) Aroclor 1248 : Congener concentrations (wt%) and comparison to published values

Congener IUPAC#	Reporting column	Co-eluting isomers	Congener Concn.	SDL	RA	RA?	S.P.D.	G.Frame	G.Fram
							wt %	wt %	wt %
190	Octyl		0.026	0.00	0.81	n		0.00	0.00
191	Octyl		0	0.00	*	n		0.00	0.00
192	Octyl		0	0.00	*	n		0.00	0.00
193	DB-1		0.009	0.00	1.33	n		0.00	0.00
194	Octyl		0.127	0.01	0.86	y		0.06	0.03
195	Octyl		0.037	0.00	1.39	n		0.02	0.01
196	Octyl		0.042	0.00	0.77	y		0.03	0.01
197	Octyl		0	0.00	*	n		0.00	0.00
198	DB-1		0	0.00	*	n		0.00	0.00
199	DB-1		0.074	0.00	0.99	y		0.09	0.05
200	Octyl		0	0.00	*	n		0.00	0.00
201	Octyl		0	0.00	*	n		0.00	0.00
202	Octyl		0.004	0.00	1.04	n		0.00	0.00
203	Octyl		0.051	0.00	0.92	y		0.05	0.02
204	Octyl		0	0.00	*	n		0.00	0.00
205	Octyl		0	0.00	*	n		0.00	0.00
206	Octyl		0	0.02	*	n		0.14	IS
207	Octyl		0	0.01	*	n		0.01	0.00
208	Octyl		0	0.01	*	n		0.06	IS
209	Octyl		0	0.00	*	n			0.00

Homologue Totals

Cl-1	0.02 wt %
Cl-2	0.82 wt %
Cl-3	27.48 wt %
Cl-4	62.48 wt %
Cl-5	16.20 wt %
Cl-6	1.96 wt %
Cl-7	0.99 wt %
Cl-8	0.34 wt %
Cl-9	0.00 wt %
Cl-10	0.00 wt %

110.29 wt %

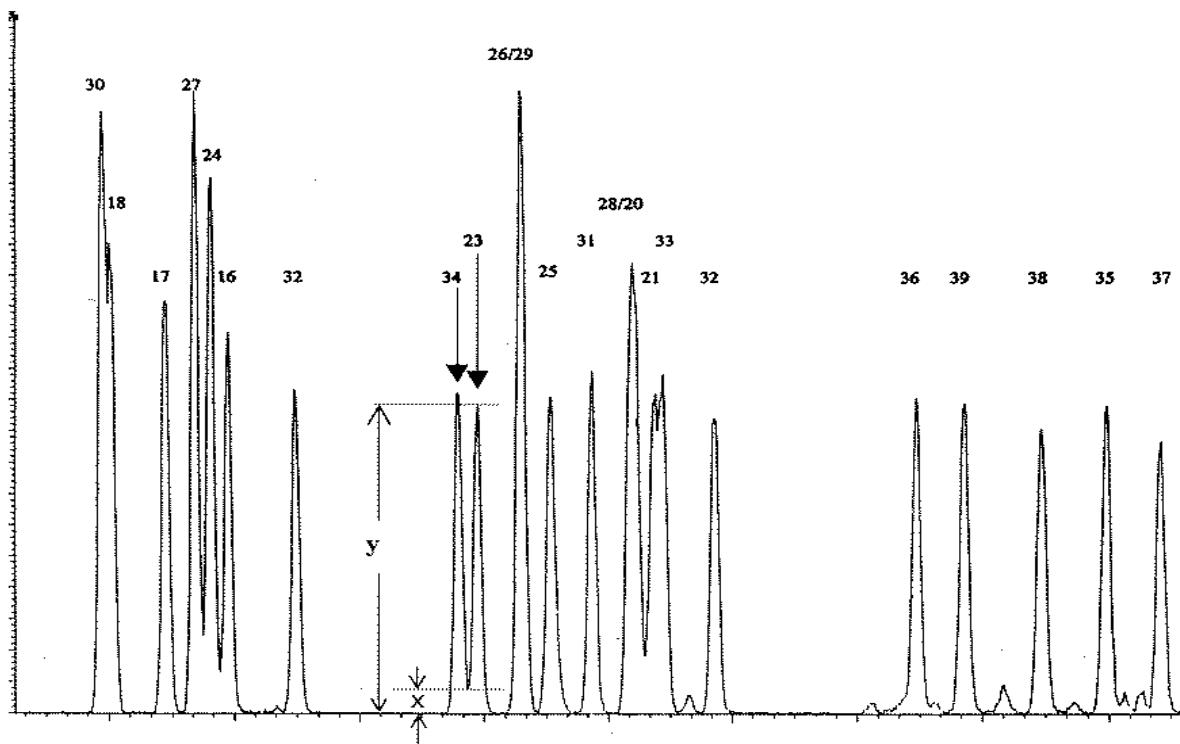


Figure 1. Octyl column resolution test #1: Separation of Cl-3 congeners 34 and 23 with valley <40% (i.e. $100x/y < 40\%$)

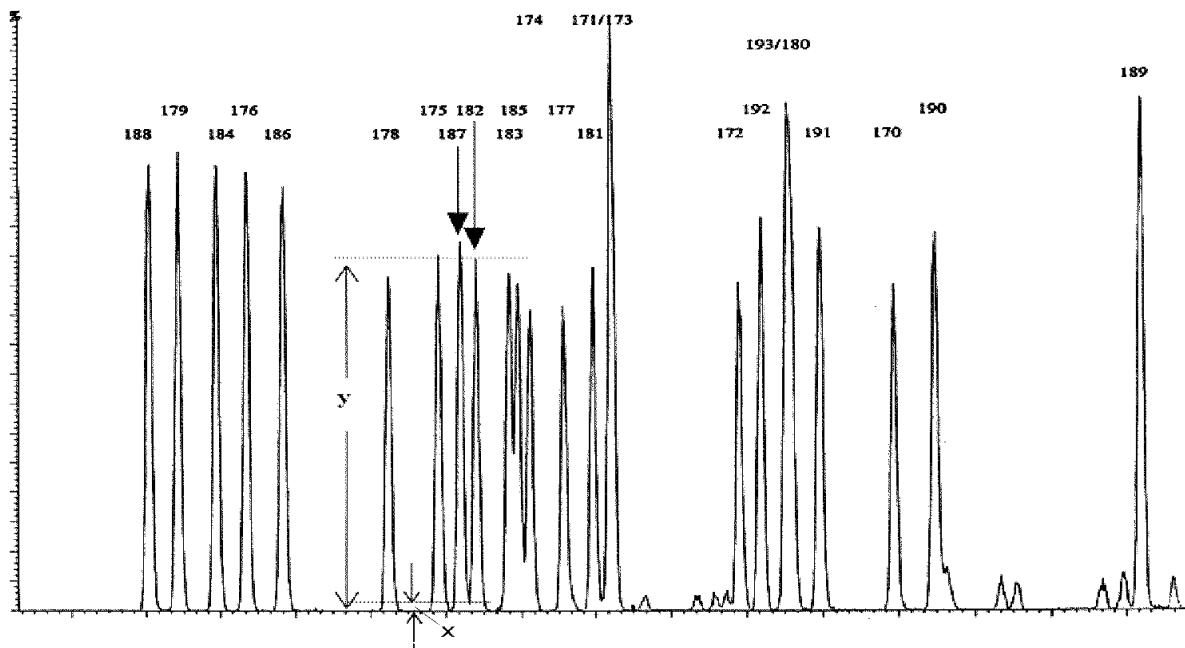


Figure 2. Octyl column resolution test #2: Separation of Cl-7 congeners 187 and 182 with valley < 40% (i.e. $100 x/y < 40\%$)